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(54) Title: A METHOD OF DESIGNING ALPHA-AMYLASE MUTANTS WITH PREDETERMINED PROPERTIES

(57) Abstract

A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least one altered property as compared to the parent α -amylase, comprises i) analysing the structure of the parent Termamyl-like α -amylase to identify at least one amino acid residue or at least one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is believed to be of relevance for altering the property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations), ii) constructing a Termamyl-like α -amylase variant, which as compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter the property, and iii) testing the resulting Termamyl-like α -amylase variant for the property in question.

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A METHOD OF DESIGNING ALPHA-AMYLASE MUTANTS WITH PREDETERMINED PROPERTIES

FIELD OF THE INVENTION

5 The present invention relates to a novel method of designing α -amylase mutants with predetermined properties, which method is based on the hitherto unknown three-dimensional structure of bacterial α -amylases.

10 BACKGROUND OF THE INVENTION

α -Amylases (α -1,4 glucan-4-glucanohydrolase, EC 3.2.1.1) constitute a group of enzymes which is capable of hydrolyzing starch and other linear and branched 1,4-glucosidic oligo- and
15 polysaccharides. Almost all α -amylases studied have a few conserved regions with approximately the same length and spacing. One of these regions resembles the Ca^{2+} binding site of calmodulin and the others are thought to be necessary for the active centre and/or binding of the substrate.

20

While the amino acid sequence and thus primary structure of a large number of α -amylases are known, it has proved very difficult to determine the three-dimensional structure of all α -amylases. The three-dimensional structure can be determined
25 by X-ray crystallographic analysis of α -amylase crystals, but it has proven difficult to obtain α -amylase crystals suitable for actually solving the structure.

Until now the three-dimensional structure of only a few
30 α -amylases have been determined at high resolution. These include the structure of the *Aspergillus oryzae* TAKA α -amylase (Swift et al., 1991), the *Aspergillus niger* acid amylase (Brady et al, 1991), the structure of pig pancreatic α -amylase (Qian et al., 1993), and the barley alpha-amylase (Kadziola et al.
35 1994, Journal of Molecular Biology 239: 104-121, A.Kadziola, Thesis, Dept of Chemistry, U. of Copenhagen, Denmark). Furthermore, the three-dimensional structure of a *Bacillus circulans* cyclodextrin glycosyltransferase (CGTase) is known

(Klein et al., 1992) (Lawson et al., 1994). The CGTase catalyzes the same type of reactions as α -amylases and exhibits some structural resemblance with α -amylases.

5 Furthermore, crystallization and preliminary X-ray studies of *B. subtilis* α -amylases have been described (Chang et al. (1992) and Mizuno et al. (1993)). No final *B. subtilis* structure has been reported. Analogously, the preparation of *B. licheniformis* α -amylase crystals has been reported (Suzuki et al. (1990), but
10 no subsequent report on X-ray crystallographic analysis or three-dimensional structure are available.

Several research teams have attempted to build three-dimensional structures on the basis of the above known
15 α -amylase structures. For instance, Vihinen et al. (J. Biochem. 107, 267-272, 1990), disclose the modelling (or computer simulation) of a three-dimensional structure of the *Bacillus stearothermophilus* α -amylase on the basis of the TAKA amylase structure. The model was used to investigate hypothetical
20 structural consequences of various site-directed mutations of the *B. stearothermophilus* α -amylase. E.A. MacGregor (1987) predicts the presence of α -helices and β -barrels in α -amylases from different sources, including barley, pig pancreas and *Bacillus amyloliquefaciens* on the basis of the known structure
25 of the *A. oryzae* TAKA α -amylase and secondary structure predicting algorithms. Furthermore, the possible loops and subsites which may be found to be present in, e.g., the *B. amyloliquefaciens* α -amylase are predicted (based on a comparison with the *A. oryzae* sequence and structure).

30

A.E. MacGregor (Starch/Stärke 45 (1993), No. 7, p. 232-237) presents a review of the relationship between the structure and activity of α -amylase related enzymes.

35 Hitherto, no three-dimensional structure has been available for the industrially important *Bacillus* α -amylases (which in the present context are termed "Termamyl-like α -amylases"),

including the *B. licheniformis*, the *B. amyloliquefaciens*, and the *B. stearothermophilus* α -amylase.

BRIEF DISCLOSURE OF THE INVENTION

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The three-dimensional structure of a Termamyl-like bacterial α -amylase has now been elucidated. On the basis of an analysis of said structure it is possible to identify structural parts or specific amino acid residues which from structural or
10 functional considerations appear to be important for conferring the various properties to the Termamyl-like α -amylases. Furthermore, when comparing the Termamyl-like α -amylase structure with known structures of the fungal and mammalian α -amylases mentioned above, it has been found that some
15 similarities exist between the structures, but also that some striking, and not previously predicted structural differences between the α -amylases exist. The present invention is based on these findings.

20 Accordingly, in a first aspect the invention relates to a method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least one altered property as compared to said parent α -amylase, which method comprises

25

i) analysing the structure of the Termamyl-like α -amylase with a view to identifying at least one amino acid residue or at least one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is
30 believed to be of relevance for altering said property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations),

ii) constructing a Termamyl-like α -amylase variant, which as
35 compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

iii) testing the resulting Termamyl-like α -amylase variant for said property.

- 5 In a second aspect the present invention relates to a method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method comprises
- 10 i) comparing the three-dimensional structure of the Termamyl-like α -amylase with the structure of a non-Termamyl-like α -amylase,
- ii) identifying a part of the Termamyl-like α -amylase structure which is different from the non-Termamyl-like α -amylase
- 15 structure, and
- iii) modifying the part of the Termamyl-like α -amylase identified in ii) whereby a Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α -amylase.

20

In a third aspect the invention relates to a method of constructing a variant of a parent non-Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method

25 comprises

- i) comparing the three-dimensional structure of the non-Termamyl-like α -amylase with the structure of a Termamyl-like α -amylase,
- ii) identifying a part of the non-Termamyl-like α -amylase
- 30 structure which is different from the Termamyl-like α -amylase structure, and
- iii) modifying the part of the non-Termamyl-like α -amylase identified in ii) whereby a non-Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the
- 35 parent Termamyl-like α -amylase.

The property which may be altered by the above methods of the present invention may, e.g., be substrate specificity,

substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6, in particular pH<5) or high (e.g. pH>9) pH values), stability towards oxidation, Ca²⁺-dependency, specific activity, and other properties of interest. For instance, the alteration may result in a variant which, as compared to the parent Termamyl-like α -amylase, has an increased specific activity at a given pH and/or an altered substrate specificity.

10

In still further aspects the invention relates to variants of a Termamyl-like α -amylase, DNA encoding such variants and methods of preparing the variants. Finally, the invention relates to the use of the variants for various industrial purposes.

15

DETAILED DISCLOSURE OF THE INVENTION

The Termamyl-like α -amylase

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It is well known that a number of alpha-amylases produced by *Bacillus* spp. are highly homologous on the amino acid level. For instance, the *B. licheniformis* α -amylase comprising the amino acid sequence shown in SEQ ID No. 2 (commercially available as Termamyl®) has been found to be about 89% homologous with the *B. amyloliquefaciens* α -amylase comprising the amino acid sequence shown in SEQ ID No. 4 and about 79% homologous with the *B. stearothermophilus* α -amylase comprising the amino acid sequence shown in SEQ ID No. 6. Further homologous α -amylases include an α -amylase derived from a strain of the *Bacillus* sp. NCIB 12289, NCIB 12512, NCIB 12513 or DSM 9375, all of which are described in detail in WO 95/26397, and the α -amylase described by Tsukamoto et al., 1988, Biochemical and Biophysical Research Communications, Vol. 151, No. 1. Still other homologous α -amylases include the α -amylase produced by the *B. licheniformis* described in EP 252 666 (ATCC 27811), and the α -amylases identified in WO 91/00353 and WO 94/18314. Other commercial Termamyl-like *B.*

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licheniformis α -amylases are Optitherm® and Takatherm® (available from Solvay), Maxamyl® (available from Gist-brocades/Genencor), Spezym AA® (available from Genencor), and Keistase® (available from Daiwa).

5

Because of the substantial homology found between these α -amylases, they are considered to belong to the same class of α -amylases, namely the class of "Termamyl-like α -amylases".

10 Accordingly, in the present context, the term "Termamyl-like α -amylase" is intended to indicate an α -amylase which, on the amino acid level, exhibits a substantial homology to Termamyl®, i.e. the *B. licheniformis* α -amylase SEQ ID NO 2. In other words, a Termamyl-like α -amylase is an α -amylase, which has the
15 amino acid sequence shown in SEQ ID No. 2, 4 or 6 herein, or the amino acid sequence shown in SEQ ID NO 1 or 2 of WO 95/26397 or in Tsukamoto et al., 1988, or i) which displays at least 60%, such as at least 70%, e.g. at least 75%, or at least 80%, e.g. at least 85%, at least 90% or at least 95% homology
20 with at least one of said amino acid sequences and/or ii) displays immunological cross-reactivity with an antibody raised against at least one of said α -amylases, and/or iii) is encoded by a DNA sequence which hybridizes to the DNA sequences encoding the above specified α -amylases which are apparent from
25 SEQ ID Nos. 1, 3 and 5 of the present application, and SEQ ID NO 4 and 5 of WO 95/26397, respectively.

In connection with property i) the "homology" may be determined by use of any conventional algorithm, preferably by use of the
30 GAP programme from the GCG package version 7.3 (June 1993) using default values for GAP penalties (Genetic Computer Group (1991) Programme Manual for the GCG Package, version 7, 575 Science Drive, Madison, Wisconsin, USA 53711).

35 Property ii) of the α -amylase, i.e. the immunological cross reactivity, may be assayed using an antibody raised against or reactive with at least one epitope of the relevant Termamyl-like α -amylase. The antibody, which may either be monoclonal or

polyclonal, may be produced by methods known in the art, e.g. as described by Hudson et al., 1989. The immunological cross-reactivity may be determined using assays known in the art, examples of which are Western Blotting or radial immunodiffusion assay, e.g. as described by Hudson et al., 1989. In this respect, immunological cross-reactivity between the α -amylases having the amino acid sequences SEQ ID Nos. 2, 4 and 6, respectively, has been found.

- 10 The oligonucleotide probe used in the characterization of the Termamyl-like α -amylase in accordance with property iii) above may suitably be prepared on the basis of the full or partial nucleotide or amino acid sequence of the α -amylase in question. Suitable conditions for testing hybridization involve
15 presoaking in 5xSSC and prehybridizing for 1h at -40°C in a solution of 20% formamide, 5xDenhardt's solution, 50mM sodium phosphate, pH 6.8, and 50 μg of denatured sonicated calf thymus DNA, followed by hybridization in the same solution supplemented with 100 μM ATP for 18h at -40°C , or other methods
20 described by e.g. Sambrook et al., 1989.

In the present context, "derived from" is intended not only to indicate an α -amylase produced or producible by a strain of the organism in question, but also an α -amylase encoded by a DNA
25 sequence isolated from such strain and produced in a host organism transformed with said DNA sequence. Finally, the term is intended to indicate an α -amylase which is encoded by a DNA sequence of synthetic and/or cDNA origin and which has the identifying characteristics of the α -amylase in question. The
30 term is also intended to indicate that the parent α -amylase may be a variant of a naturally occurring α -amylase, i.e. a variant which is the result of a modification (insertion, substitution, deletion) of one or more amino acid residues of the naturally occurring α -amylase.

Parent hybrid α -amylases

The parent α -amylase (being a Termamyl-like or non-Termamyl-like α -amylase) may be a hybrid α -amylase, i.e. an α -amylase
5 which comprises a combination of partial amino acid sequences derived from at least two α -amylases.

The parent hybrid α -amylase may be one which on the basis of amino acid homology and/or immunological cross-reactivity
10 and/or DNA hybridization (as defined above) can be determined to belong to the Termamyl-like α -amylase family. In this case, the hybrid α -amylase is typically composed of at least one part of a Termamyl-like α -amylase and part(s) of one or more other α -amylases selected from Termamyl-like α -amylases or non-
15 Termamyl-like α -amylases of microbial (bacterial or fungal) and/or mammalian origin.

Thus, the parent hybrid α -amylase may comprise a combination of at least two Termamyl-like α -amylases, or of at least one
20 Termamyl-like and at least one non-Termamyl-like bacterial α -amylase, or of at least one Termamyl-like and at least one fungal α -amylase. For instance, the parent α -amylase comprises a C-terminal part of an α -amylase derived from a strain of *B. licheniformis* and a N-terminal part of an α -amylase derived
25 from a strain of *B. amyloliquefaciens* or from a strain of *B. stearothermophilus*. For instance, the parent α -amylase comprises at least 430 amino acid residues of the C-terminal part of the *B. licheniformis* α -amylase, and may, e.g. comprise
a) an amino acid segment corresponding to the 37 N-terminal
30 amino acid residues of the *B. amyloliquefaciens* α -amylase having the amino acid sequence shown in SEQ ID No. 4 and an amino acid segment corresponding to the 445 C-terminal amino acid residues of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2, or b) an amino acid
35 segment corresponding to the 68 N-terminal amino acid residues of the *B. stearothermophilus* α -amylase having the amino acid sequence shown in SEQ ID No. 6 and an amino acid segment corresponding to the 415 C-terminal amino acid residues of the

B. licheniformis α -amylase having the amino acid sequence shown in SEQ ID No. 2.

Analogously, the parent hybrid α -amylase may belong to a non-Termamyl-like α -amylase family, e.g. the Fungamyl-like α -amylase family. In that case the hybrid may comprise at least one part of an α -amylase belonging to the non-Termamyl-like α -amylase family in combination with one or more parts derived from other α -amylases.

10

The three-dimensional Termamyl-like α -amylase structure

The Termamyl-like α -amylase which was used to elucidate the three-dimensional structure forming the basis for the present invention consists of the 300 N-terminal amino acids of the *B. amyloliquefaciens* α -amylase (with the amino acid sequence shown in SEQ ID No. 4) and amino acids 301-483 of the C-terminal end of the *B. licheniformis* α -amylase with the amino acid sequence SEQ ID No. 2. The bacterial α -amylase belongs to the "Termamyl-like α -amylase family" and the present structure is believed to be representative for the structure of any Termamyl-like α -amylase.

The structure of the α -amylase was solved in accordance with the principle for X-ray crystallographic methods given in "X-Ray Structure Determination", Stout, G.K. and Jensen, L.H., John Wiley & Sons, inc. NY, 1989. The structural coordinates for the solved crystal structure of the α -amylase at 2.2 Å resolution using the isomorphous replacement method are given in a standard PDB format (Brookhaven Protein Data Base) in Appendix 1. It is to be understood that Appendix 1 forms part of the present application.

Amino acid residues of the enzyme are identified by three-letter amino acid code (capitalized letters).

The α -amylase structure is made up of three globular domains ordered A, B, and C with respect to sequence, which lie

approximately along a line in the order B, A, C. The domains can be defined as being residues 1-103 and 206-395 for domain A, residues 104-205 for domain B, and residues 396-483 for domain C, the numbers referring to the *B. licheniformis* α -amylase. This gives rise to an elongated molecule, the longest axis being about 85Å. The widest point perpendicular to this axis is approximately 50Å and spans the central A domain. The active site residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) are D323, D231 and E261.

10

Domain A

Domain A is the largest domain and contains the active site (comprised of a cluster of three amino acid residues placed at the bottom of a deep cleft in the enzyme's surface). Domain A of all known α -amylase structures have the same overall fold, viz. the (beta/alpha)₈ barrel with 8 central beta strands (number 1-8) and 8 flanking α -helices. The β -barrel is defined by McGregor op. cit. The C-terminal end of Beta strand 1 is connected to helix 1 by a loop denoted loop 1 and an identical pattern is found for the other loops. These loops show some variation in size and some can be quite extensive.

The 8 central Beta-strands in the (beta/alpha)₈ barrel superimpose well between the various known α -amylase structures, and this part of the structure, including the close surroundings of the active site located at the c-terminal end of the beta-strands, show high similarity between the different amylases.

30

The loops connecting beta-strands and alpha helices display high variations between alpha amylases. These loops constitute the structural context of the active site and the majority of the contacts to the substrate is found among residues located in these loops. Such important characteristics as substrate specificity, substrate binding, pH/activity profile, starch cleavage pattern are determined by the amino acids and the positions of same in these loops.

The substantial differences between the Fungamyl-like α -amylase structure and the structure of the Termamyl-like α -amylase disclosed herein which are found in loops 1, 2, 3, and 8 are visualized in the Figures.

5

Domain B

The Termamyl-like α -amylase structure has been found to comprise a special domain structure in the A domain's loop3, also called domain B. The structure of the Termamyl-like α -amylase B domain has never been seen before in any of the known α -amylase or $(\beta/\alpha)_8$ -barrel proteins.

The domain B structure is a very compact domain having a very high number of charged residues. The B domain arises as an extension of the loop between strand 3 and helix 3 of domain A (shown in Fig. 7) and contains a 5 stranded antiparallel β -sheet structure containing at least one long loop structure and having the connectivity -1, +3, -1X, +2 (Richardson, 1981, Adv. Protein Chem. 34, 167-339).

The first four strands of the B domain form two hairpin loops which twist around each other like a pair of crossed fingers (right-hand twist). The mainchain folds into a β -strand which connects two small β -sheet structures. After making one turn in one sheet it folds back and makes up a two stranded sheet in contact with domain A and an internal hole in the α -amylase structure. Then the mainchain folds up to a small sheet structure nearly perpendicular to the first two sheets. Before entering the helix 3 on top of the β -strand 3, the approximately 24 last amino acids in domain B form two calcium binding sites in the contact region to domain A.

Domain B is connected with domain A by two peptide stretches, which divide the domain-domain contact areas into two. Domain B is in contact with Domain A by a calcium binding region and an internally buried hole containing waters. Many types of molecular contacts are present. Ionic interacting between acid

and basic amino acids are possible, these interactions are very important for the general stability at high pH and for keeping the Calcium binding sites intact.

5 *Domain C*

Domain C is the C-terminal part of the protein consisting of amino acids 394-483. Domain C is composed entirely of β -strands which forms a single 8-stranded sheet structure, which folds
10 back on itself, and thus may be described as a β -sandwich structure. The connectivity is +1,+1, +5, -3, +1, +1, -3 although strands 6 and 7 are only loosely connected. One part of the β -sheet forms the interface to domain A.

15 *Ca-binding and Na-binding sites*

The structure of the Termamyl-like α -amylase is remarkable in that it exhibits four calcium-binding sites and one sodium-binding site. In other words four calcium ions and one sodium
20 ion are found to be present in the structure, although one of the calcium ions displays very weak coordination. Two of the calcium ions form part of a linear cluster of three ions, the central ion being attributed to sodium, which lie at the junction of the A and B domains.

25

The coordinating residues for the calcium ions between the A and B domain are as follows (using the Pdb file nomenclature for amino acid residues and atoms in the Pdb file found in Appendix 1 herein): For the calcium ion nearest to the active
30 site (IUM 502 in the pdb file), the backbone carbonyls from His235 and Asp194, the sidechain atom OD1 from residues Asp194, Asn102 and Asp200, and one water molecule WAT X3 (atom OW7). For the sodium ion (IUM 505), the binding site includes atom OD2 from Asp194, Asp200, Asp183 and Asp159, and a backbone
35 carbonyl from Val201. The coordinates for the other calcium ion between domain A and B are (IUM 501) : atom OD2 from Asp204 and Asp159, backbone carbonyl from Asp183 and Ala181, atom OD1 from Asp202, and one water molecule WAT X7 (atom OW7).

One calcium ion is located between the A and C domain, another is located in the C domain. The first mentioned calcium ion, which is also the one best coordinated (IUM 503) includes a carbonyl backbone from Gly300, Tyr302 and His406, atom OD2/OD1 from Asp430, atom OD1 from Asp407, and one water molecule WAT X6 (atom OW7). The other and very weakly coordinated calcium site (IUM 504) comprises 4 water molecules WAT X21 (atom OW8), X6 (atom OW6), X9 (atom OW0) and X28 (atom OW8), OE1/OE2 from Glu447 and OD1 from Asn444.

Substrate-binding site

Without being limited to any theory it is presently believed that favourable interactions between a substrate molecule and the enzyme (such as hydrogen bonds and/or strong electrostatic interaction) are found within a sphere of 4Å of the substrate, when bound to the enzyme. The following residues of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2 are contemplated to be within a distance of 4 Å of the substrate and thus believed to be involved in interactions with the substrate:

Trp13, Tyr14, Asn17, Asp18, Ser50, Gln51, Ala52, Asp53, Val54, Gly55, Tyr56, Lys70, Arg74, Lys76, Val102, His105, Gly107, Gly108, Ala109, Trp138, Thr163, Asp164, Trp165, Asn172, Glu189, Tyr193, Leu196, Met197, Tyr198, Ala199, Arg229, Asp231, Ala232, Lys234, His235, Glu261, Trp263, His327, Asp328, Gln333, Ser334, and Leu335.

The amino acid residues of another Termamyl-like α -amylase, which are contemplated to be within a distance of 4Å of the substrate, may easily be identified by aligning the amino acid sequence SEQ ID NO 2 with that of the other Termamyl-like α -amylase and thereby identifying the positions equivalent to those identified above.

Generality of structure

Because of the high homology between the various Termamyl-like α -amylases, the solved structure defined by the coordinates of Appendix 1 is believed to be representative for the structure of all Termamyl-like α -amylases. A model structure of other Termamyl-like α -amylases may easily be built on the basis of the coordinates given in Appendix 1 adapted to the α -amylase in question by use of an alignment between the respective amino acid sequences. The creation of a model structure is exemplified in Example 1.

The above identified structurally characteristic parts of the Termamyl-like α -amylase structure (Ca-binding site, substrate binding site, loops, etc.) may easily be identified in other Termamyl-like α -amylases on the basis of a model (or solved) structure of the relevant Termamyl-like α -amylase or simply on the basis of an alignment between the amino acid sequence of the Termamyl-like α -amylase in question with that of the *B. licheniformis* α -amylase used herein for identifying the amino acid residues of the respective structural elements.

Furthermore, in connection with Termamyl-like variants of the invention, which are defined by modification of specific amino acid residues of a specific Termamyl-like α -amylase, it will be understood that variants of another Termamyl-like α -amylase modified in an equivalent position (as determined from the best possible amino acid sequence alignment between the respective sequences) are intended to be covered as well. Thus, irrespective of whether an amino acid residue is identified herein for the purpose of defining a structural part of a given α -amylase or used for identifying a variant of the α -amylase, this amino acid residue shall be considered as representing the equivalent amino acid residue of any other Termamyl-like α -amylase.

Methods of the invention for design of novel α -amylase variants

In the methods according to the first, second and third aspects of the invention the terms "structure of a Termamyl-like α -amylase" and "Termamyl-like α -amylase structure" are intended to indicate the solved structure defined by the coordinates presented in Appendix 1 or a model structure of a given Termamyl-like α -amylase (such as the *B. licheniformis* α -amylase) built on the basis of the solved structure.

10

In most cases the parent Termamyl-like α -amylase to be modified in accordance with the present invention is different from the α -amylase which was actually used for solving the structure (Appendix 1). This means that the amino acid residue(s) or structural part(s) identified in the solved structure (Appendix 1) in step i) of the method according to the first, second or third aspect of the invention must be translated into the corresponding amino acid residue(s) or structural part(s) of the parent Termamyl-like α -amylase in question. The "translation" is conveniently performed on the basis of an amino acid sequence alignment between the amino acid sequence of the Termamyl-like α -amylase used for solving the structure and the amino acid sequence of the parent Termamyl-like α -amylase in question.

25

The analysis or comparison performed in step i) of the method according to the first, second and third aspect, respectively, of the invention may be performed by use of any suitable computer programme capable of analysing and/or comparing protein structures, e.g. the computer programme Insight, available from Biosym Technologies, Inc. For instance, the basic principle of structure comparison is that the three-dimensional structures to be compared are superimposed on the basis of an alignment of secondary structure elements (such as the central 8 β -strands in the barrel) and the parts differing between the structures can subsequently easily be identified from the superimposed structure.

35

The structural part which is identified in step i) of the methods of the first, second and third aspects of the invention may be composed of one amino acid residue. However, normally the structural part comprises more than one amino acid residue, typically constituting one of the above parts of the Termamyl-like α -amylase structure such as one of the A, B, or C domains, an interface between any of these domains, a calcium binding site, a loop structure, the substrate binding site, or the like.

10

In the present context the term "structural or functional considerations" is intended to indicate that modifications are made on the basis of an analysis of the relevant structure or structural part and its contemplated impact on the function of the enzyme. Thus, an analysis of the structures of the various α -amylases, which until now has been elucidated, optionally in combination with an analysis of the functional differences between these α -amylases, may be used for assigning certain properties of the α -amylases to certain parts of the α -amylase structure or to contemplate such relationship. For instance, differences in the pattern or structure of loops surrounding the active site may result in differences in access to the active site of the substrate and thus differences in substrate specificity and/or cleavage pattern. Furthermore, parts of a Termamyl-like α -amylase involved in or contemplated to be involved in substrate binding (and thus e.g. specificity/cleavage pattern), calcium or sodium ion binding (e.g. of importance for the Calcium-dependency of the enzyme), and the like has been identified (*vide infra*).

30

The modification of an amino acid residue or structural part is typically accomplished by suitable modifications of a DNA sequence encoding the parent enzyme in question. The term "modified" as used in step ii) in the method according to the first aspect of the invention is intended to have the following meaning: When used in relation to an amino acid residue the term is intended to mean replacement of the amino acid residue in question with another amino acid residue. When used in

relation to a structural part, the term is intended to mean replacement of one or more amino acid residues of said structural part, addition of one or more amino acid residues to said part, or deletion of one or more amino acid residues of
5 said structural part.

The construction of the variant of interest is accomplished by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing
10 the variant, and optionally subsequently recovering the variant from the resulting culture broth. This is described in detail further below.

First aspect of the invention

15 In a preferred embodiment of the method according to the first aspect of the invention the property of the parent enzyme to be modified is selected from calcium dependency, substrate binding, cleavage pattern, pH dependent activity and the like. Specific examples of how to change these properties of a parent
20 Termamyl-like α -amylase are given further below.

In another preferred embodiment the parent Termamyl-like α -amylase to be modified is a *B. licheniformis* α -amylase.

25 *Second and third aspects of the invention*

One important advantage of the methods according to the second and third aspects of the present invention is that it is possible to adapt the structure (or a structural part) of a Termamyl-like α -amylase to the structure (or structural part)
30 of a non-Termamyl-like α -amylase and *vide versa*. For instance, having identified a loop structure of the non-Termamyl-like α -amylase which is believed to be responsible for or contributing to a particular property of the non-Termamyl-like α -amylase it is possible to replace the corresponding structure of the
35 Termamyl-like α -amylase with said non-Termamyl-like α -amylase structure - or if no corresponding structure exists in the Termamyl-like α -amylase - to insert the structure into the Termamyl-like α -amylase in such a manner that the resulting

variant Termamyl-like α -amylase, as far as the relevant part is concerned, resembles the corresponding part of the non-Termamyl-like α -amylase. When two or more parts of the structure of the parent Termamyl-like α -amylase are modified so
5 as to resemble the corresponding parts of the non-Termamyl-like α -amylase it is possible to increase the resemblance to the non-Termamyl-like α -amylase of the Termamyl-like α -amylase variant and thus to alter the properties of said variant in the direction of those of said non-Termamyl-like α -amylase. Loop
10 modifications are discussed in much further detail further below.

Typically, the modification to be performed in step iii) of the method according to the second aspect of the invention is
15 accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified so as to adapt the structure of said part of the parent α -amylase to the corresponding part of the non-Termamyl-like α -amylase; by replacing one or more amino acid residues of the part of the
20 Termamyl-like α -amylase to be modified with the amino acid residues occupying corresponding positions in the non-Termamyl-like α -amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α -amylase into a corresponding position in the Termamyl-like α -amylase. For the
25 method according to the third aspect the modification is to be understood analogously, performed on the non-Termamyl-like parent α -amylase rather than the Termamyl-like α -amylase.

In step ii) of the method according to the second or third
30 aspect of the invention the part of the structure to be identified is preferably one which in the folded enzyme is believed to be in contact with the substrate (cf the disclosure above in the section entitled "Substrate-binding site) or involved in substrate specificity and/or cleavage pattern,
35 and/or one which is in contact with one of the calcium or sodium ions and/or one, which is contributing to the pH or temperature profile of the enzyme, or one which otherwise, from structural or functional considerations, is contemplated to be

responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α -amylase.

Non-Termamyl-like α -amylase

5 The non-Termamyl-like α -amylase with which the comparison is made in step i) of the method of the second aspect of the invention and which is the parent α -amylase in the method of the third aspect of the invention, may be any α -amylase, which does not belong to the family of Termamyl-like α -amylases (as
10 defined above) and, which as a consequence thereof, has a different three-dimensional structure. Furthermore, the non-Termamyl-like α -amylase should be one which has, at the time that the method is performed, an elucidated or contemplated three-dimensional structure.

15

The non-Termamyl-like α -amylase may, e.g., be a fungal α -amylase, a mammalian or a plant α -amylase or a bacterial α -amylase (different from a Termamyl-like α -amylase). Specific examples of such α -amylases include the *Aspergillus oryzae* TAKA
20 α -amylase, the *A. niger* acid α -amylase, the *Bacillus subtilis* α -amylase, the porcine pancreatic α -amylase and a barley α -amylase. All of these α -amylases have elucidated structures which are clearly different from the structure of the Termamyl-like α -amylase shown herein.

25

The fungal α -amylases mentioned above, i.e. derived from *A. niger* and *A. oryzae*, are highly homologous on the amino acid level and generally considered to belong to the same family of α -amylases. In the present disclosure, this family is termed
30 "Fungamyl-like α -amylase" and intends to indicate an α -amylase which exhibits a high homology, i.e. more than 70%, such as 80% homologous (as defined herein) to the fungal α -amylase derived from *Aspergillus oryzae*, commercially available as Fungamyl[®], and the *A. niger* α -amylase.

35

From the enclosed illustrations of the α -amylase structure of a Termamyl-like α -amylase and a comparison of said structure with the structure of a Fungamyl-like α -amylase it is evident

that major differences exist between the two structures. In the method of the invention it is of particular interest to modify parts of the parent Termamyl-like α -amylase, which belong to a region with large differences to the Fungamyl-like α -amylase. In particular, it is of interest to modify the parent Termamyl-like α -amylase in one or more of the following loops: loop 1, loop 2, loop 3 and/or loop 8 of the parent α -amylase.

In the method of the third aspect of the invention it is of particular interest to modify loop 1, loop 2, loop 3 and/or loop 8 of the parent non-Termamyl-like α -amylase to a closer resemblance to the similar loops of a Termamyl-like α -amylase, such as Termamyl.

In the following specific types of variants are described which have been designed by use of the method of the invention.

Loop modifications

In order to change the substrate specificity of the parent α -amylase to be modified it is relevant to consider loop modifications. For instance changing one or more of the loop structures of the Termamyl-like α -amylase into a closer resemblance with the corresponding loop structure(s) of a non-Termamyl-like α -amylase (such as a Fungamyl-like α -amylase) it is contemplated that it is possible to change the substrate specificity in the direction of that of the non-Termamyl α -amylase. In the following different types of loop modifications of interest are listed. It will be understood that the variants may have other changed properties in addition to the modified substrate specificity. It will be understood that the following modifications identified for a specific Termamyl-like α -amylase are intended to include corresponding modifications in other equivalent positions of other Termamyl-like α -amylases. Furthermore, it will be understood that, normally, the loop modification will comprise replacement of an entire loop structure or a substantial part thereof in, e.g., the Termamyl-

like α -amylase, with the corresponding loop structure (or substantial part thereof) in a non-Termamyl-like α -amylase.

Loop2 modifications

5 In one embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one amino acid residue of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ ID No. 4, i.e. loop 2,
10 has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No.
15 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

The amino acid sequence shown in SEQ ID No. 10 is the amino acid sequence of the *A. oryzae* α -amylase, i.e. a Fungamyl-like
20 α -amylase. It will be understood that amino acid residues or fragments found in corresponding positions in other α -amylases, in particular Fungamyl-like α -amylases, may be used as a template for the construction of the variant according to the invention. The corresponding part in other homologous α -
25 amylases may easily be identified on the basis of a comparison of the amino acid sequences and/or three-dimensional structures of the respective α -amylases.

For instance, the variant may be one, which, when the amino
30 acid sequence of the variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% such as at least 90% sequence homology with the part of SEQ ID No 10 extending
35 from residue Z to residue V of SEQ ID No 10, wherein
X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,
Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and
5 V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

In other words, the variant may be one in which an amino acid fragment X-Y of the parent α -amylase, which corresponds to or
10 is within the amino acid fragment 44-57 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, in X, Y, Z and V have the meaning indicated above.

15

A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α -amylase, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 48-51 of SEQ ID No. 4, has been replaced
20 with an amino acid fragment corresponding to amino acid residues 70-78 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - limited alteration

25 In another embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 195-202 of the amino acid sequence of SEQ
30 ID No. 4, has been deleted or replaced with one or more of the amino acid residues which is/are present in an amino acid fragment corresponding to the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the
35 relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one in which an amino acid fragment X-Y of the parent α -amylase which corresponds to or is within the amino acid fragment 195-202 of SEQ ID No. 4, has been replaced by an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, in which

X is an amino acid residue corresponding to the amino acid occupying position 195 or 196 of SEQ ID No. 4,

10

Y is an amino acid residue corresponding to the amino acid occupying position 198, 199, 200, 201, or 202 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 165 or 166 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 173, 174, 175, 176 or 177 of SEQ ID No. 10.

Expressed in another manner, the variant according to this aspect may be one, which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent Termamyl-like α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, the meaning of X, Y, Z and V being as identified above.

A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α -amylase, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - complete domain B

In a further embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which
5 is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino
10 acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

15 For instance, the variant may be one, in which an amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-210 of
20 the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,
25

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and
30

V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

A specific example of a variant according to this embodiment is
35 a variant of a parent α -amylase, in which an amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with

the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

In another embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-177 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-202 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

A specific example of a variant according to this embodiment of the invention is a variant, in which the amino acid fragment of

the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

5

Loop 1 modifications - minimal addition

In a further embodiment the present invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -
10 amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to
15 the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

20 For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 12-19 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 28-42 of
25 the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

30

Y is an amino acid residue corresponding to the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid
35 occupying position 28, 29, 30, 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

A specific example of a variant according to this aspect of the invention is a variant, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

Loop 1 modifications - complete loop

In a further embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 7-23 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 13-45 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

A specific variant according to this embodiment is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

10

Loop 8 modifications

In a further embodiment the invention relates to a variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 322-346 of SEQ ID No. 2, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 291-313 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

35

Y is an amino acid residue corresponding to the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is an amino acid residue corresponding to the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

A specific variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

Ca²⁺ dependency

It is highly desirable to be able to decrease the Ca²⁺ dependency of a Termamyl-like α -amylase. Accordingly, in a further aspect the invention relates to a variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a decreased Ca²⁺ dependency as compared to the parent α -amylase. The decreased Ca²⁺ dependency has the functional result that the variant exhibits a satisfactory amylolytic activity in the presence of a lower concentration of calcium ion in the extraneous medium than is necessary for the parent enzyme and, for example, therefore is less sensitive than the parent to calcium ion-depleting conditions such as those obtained in media containing calcium-complexing agents (such as certain detergent builders).

The decreased Ca²⁺ dependency of the variant of the invention may advantageously be achieved by increasing the Ca²⁺ binding affinity of the parent Termamyl-like α -amylase, in other words the stronger the Ca²⁺ binding of the enzyme, the lower is the Ca²⁺ dependency.

It is presently believed that amino acid residues located within 10Å from a sodium or calcium ion are involved in or are of importance for the Ca²⁺ binding capability of the enzyme.

Accordingly, the variant according to this aspect of the invention is preferably one, which has been modified in one or more amino acid residues present within 10Å from a calcium and/or sodium ion identified in the three-dimensional Termamyl-like α -amylase structure in such a manner that the affinity of the α -amylase for calcium is increased.

The amino acid residues found within a distance of 10Å from the Ca^{2+} binding sites of the *B. licheniformis* α -amylase with the amino acid sequence SEQ ID NO 2 were determined as described in Example 2 and are as follows:

V102, I103, N104, H105, K106, R125, W155, W157, Y158, H159, F160, D161, G162, T163, Y175, K176, F177, G178, K180, A181, W182, D183, W184, E185, V186, S187, N192, Y193, D194, Y195, L196, M197, Y198, A199, D200, I201, D202, Y203, D204, H205, P206, V208, A209, D231, A232, V233, K234, H235, I236, K237, F238, F240, L241, A294, A295, S296, T297, Q298, G299, G300, G301, Y302, D303, M304, R305, K306, L307, W342, F343, L346, Q393, Y394, Y396, H405, H406, D407, I408, V409, R413, E414, G415, D416, S417, V419, A420, N421, S422, G423, L424, I428, T429, D430, G431, P432, V440, G441, R442, Q443, N444, A445, G446, E447, T448, W449, I462, G475, Y480, V481, Q482, R483.

In order to construct a variant according to this aspect of the invention it is desirable to replace at least one of the above mentioned amino acid residues (or an amino acid residue occupying an equivalent position in another Termamyl-like α -amylase than that defined by SEQ ID NO 2), which is contemplated to be involved in providing a non-optimal calcium binding, with any other amino acid residue which improves the Ca^{2+} binding affinity of the variant enzyme. In practice, the identification and subsequent modification of the amino acid residue is performed by the following method:

i) identifying an amino acid residue within 10Å from a Ca^{2+} binding site of a Termamyl-like α -amylase structure, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,

ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and testing the Ca^{2+} dependency of the resulting Termamyl-like α -amylase variant.

10 In the present context, the term "non-optimal calcium ion interaction" is intended to indicate that the amino acid residue in question is selected on the basis of a presumption that substituting said amino acid residue for another may improve a calcium ion binding interaction of the enzyme. For
15 instance, the amino acid residue in question may be selected on the basis of one or more of the following considerations:

- to obtain an improved interaction between a calcium ion and an amino acid residue located near to the surface of the enzyme
20 (as identified from the structure of the Termamyl-like α -amylase). For instance, if the amino acid residue in question is exposed to a surrounding solvent, it may be advantageous to increase the shielding of said amino acid residue from the solvent so as to provide for a stronger interaction between
25 said amino acid residue and a calcium ion. This can be achieved by replacing said residue (or an amino acid residue in the vicinity of said residue contributing to the shielding) by an amino acid residue which is more bulky or otherwise results in an improved shielding effect.

30

- to stabilize a calcium binding site, for instance by stabilizing the structure of the Termamyl-like α -amylase (e.g. by stabilizing the contacts between the A, B and C domains or stabilizing one or more of the domains as such). This may,
35 e.g., be achieved by providing for a better coordination to amino acid side chains, which may, e.g., be obtained by replacing an N residue with a D residue and/or a Q residue with

an E residue (e.g. N104D), e.g. within 10Å, and preferably within 3 or 4Å, of a calcium binding site.

- to protect the calcium binding site or to improve the coordination between the calcium ion and the calcium binding site, e.g. by providing a stronger interaction between the ion and the binding site.

Before actually constructing a Termamyl-like α -amylase variant according to the above principles it may be convenient to evaluate the contemplated amino acid modification by its accommodation into the Termamyl-like α -amylase structure, e.g. into a model structure of the parent Termamyl-like α -amylase.

Preferably, the amino acid residue to be modified is located within 8Å of a Ca^{2+} binding site residue, such as within 5Å of such residue. The amino acid residues within 8Å and 5Å, respectively, may easily be identified by an analogous method used for identifying amino acid residues within 10Å (cf. Example 2).

The following mutation is contemplated to be of particular interest with respect to decreasing the Ca^{2+} dependency of a Termamyl-like α -amylase:

N104D (of the *B. licheniformis* α -amylase SEQ ID NO 2, or an equivalent (N to D) mutation of an equivalent position in another Termamyl-like α -amylase.)

In connection with substitutions of relevance for Ca^{2+} dependency, some other substitutions appear to be of importance in stabilizing the enzyme conformation (for instance the Domains A-B and/or Domains A-C interactions contributing to the overall stability of the enzyme) in that they may, e.g., enhance the strength of binding or retention of calcium ion or sodium ion at or within a calcium or sodium binding site, respectively, within the parent Termamyl-like α -amylase.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

A. CLASSIFICATION OF SUBJECT MATTER

IPC6: C12N 9/28, C12N 15/56

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC6: C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPI, CA, MEDLINE, BIOSIS

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	Dialog Information Services, File 5, BIOSIS PREVIEWS, Dialog accession no. 11619266, BIOSIS no. 98219266, Machius M et al: "Crystal structure of calcium-depleted Bacillus licheni- formis alpha-amylase at 2.2 A resolution", & Journal of Molecular Biology 246 (4). 1995. 545-559	1-17
	--	
X	Dialog Information Services, file 155, MEDLINE, Dialog accession no. 08974640, MEDLINE accession no. 94289640, Svensson B: "Protein engineering in the alpha-amylase family: catalytic mechanism, substrate specificity, and stability", & Plant Mol Biol (NETHERLANDS) May 1994, 25 (2) p141-57	1-17
	--	

☒ Further documents are listed in the continuation of Box C.☒ See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search

5 July 1996

Date of mailing of the international search report

05 -07- 1996

Name and mailing address of the ISA

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The invention claimed relates to a method of constructing alpha-amylase variants with predetermined properties by comparing the three-dimensional structures of enzymes. The claims also include many alpha-amylase variants.

"A search for a special technical feature" as mentioned in PCT Rule 13.2 among the independent claims did not reveal a unifying, novel technical feature.

Accordingly, the following inventions were found:

- I Claims 1-17 focus on a method of constructing alpha-amylase variants by comparing the three-dimensional structure of a parent enzyme (Ternary-like alpha-amylase) with another enzyme e.g. mammalian or fungal alpha-amylases. The differences in structure are compared with the differences in function, whereafter new variants with new predictable characteristics are produced.
- II Claims 45-46 directed to a alpha-amylase variant that has decreased Ca^{2+} dependency,
- III Claim 47 directed to a alpha-amylase variant that exhibits higher activity below the pH-optimum than the parent enzyme.
- IV Claim 48 directed to a alpha-amylase variant having an increased thermostability and/or altered temperature optimum.
- V Claim 50 directed to a variant having reduced capability of cleaving an oligo-saccharide substrate close to its branching point.

Due to the complex construction of the claims and the fact that the search so far has not covered all aspects of the invention, it may be that further non-unity remarks can appear. If further searches are done, references might appear which will give further a posteriori non-unity remarks.

Therefore, the search has been restricted to the first invention.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

Claims 18-43 are directed to a number of different variants that are composed of several inventions. They are, however, so complex and broad that no meaningful search can be done, especially as no special characteristic is linked to the groups of variants. It is for example unlikely that claim 18 concerns one invention. It is not believable that a change in any amino acid in one fragment for one/or none of the amino acids in a fragment of another enzyme gives an enzyme with the same new and valuable characteristic. The formulation of claims 18-43 is so complicated because of all the different combinations of amino acid substitutions.

Thus they do not comply with Art. 6. PCT prescribing that claims shall be clear and concise.

2
INTERNATIONAL SEARCH REPORT

International application No.
PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	Dialog Information Services, file 155, MEDLINE. Dialog accession no. 08958150, MEDLINE accession no. 94273150, Nakatani H et al: "Effect of modifying histidine residues on the action of Bacillus amylo- liquefaciens and barley-malt alpha-amylases", & Carbohydr Res (NETHERLANDS) Apr 16 1994, 257 (1) p 155-61	1-17
Y	--	45-46
X	J. MED. BIOL., Volume 229, 1993, C. Chang et al, "Crystallization and Preliminary X-ray Crystallographic Analysis of alpha-Amylase from Bacillus subtilis" page 235 - page 238	1-17
	--	
A	WO 9100343 A2 (GIST-BROCADES N.V.), 10 January 1991 (10.01.91)	1-17
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A	EP 0410498 A2 (GIST-BROCADES N.V.), 30 January 1991 (30.01.91)	1-17
	--	
A	JOURNAL OF BACTERIOLOGY, Volume 166, No 2, May 1986, G. L. Gray et al, "Structural Genes Encoding the Thermophilic alpha-Amylases of Bacillus stearothermophilus and Bacillus licheniformis" page 635 - page 643	1-17
	--	
P,X	WO 9535382 A2 (GISTBROCADES B.V.), 28 December 1995 (28.12.95), claims 1-2, abstract	45-46
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Y	WO 9418314 A1 (GENENCOR INTERNATIONAL), 18 August 1994 (18.08.94)	45-46
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INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	<p>Chemical Abstracts, Volume 108, No 11, 14 March 1988 (14.03.88), (Columbus, Ohio, USA), Buisson, G. et al, "Three dimensional structure of porcine pancreatic alpha-amylase at 2.9 Å resolution. Role of calcium in structure and activity", page 325, THE ABSTRACT No 90927h, EMBO J. 1987, 6 (13), 3909-3916</p> <p style="text-align: center;">--</p>	45-46
Y	<p>Chemical Abstracts, Volume 112, No 15, 9 April 1990 (09.04.90), (Columbus, Ohio, USA), Vihinen, Mauno et al, "Site-directed mutagenesis of a thermostable alpha-amylase from Bacillus stearothermophilus: putative role of three conserved residues", page 347, THE ABSTRACT No 135178r, J. Biochem 1990, 107 (2), 267-272</p> <p style="text-align: center;">--</p>	45-46
A	<p>US 4600693 A (KAREN L. KINDLE ET AL), 15 July 1986 (15.07.86)</p> <p style="text-align: center;">--</p>	45-46
A	<p>Chemical Abstracts, Volume 112, No 19, 7 May 1990 (07.05.90), (Columbus, Ohio, USA), Holm, Liisa et al, "Random mutagenesis used to probe the structure and function of Bacillus stearothermophilus alpha-amylase", page 351, THE ABSTRACT No 174785f, Protein Eng. 1990, 3 (3), 181-191</p> <p style="text-align: center;">-- -----</p>	45-46

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK96/00057

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

see next sheet

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see next sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☒ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
Claims 1-17 directed to a method of constructing alpha-amylase variants and claims 45-46 directed to an alpha-amylase.
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
☒ No protest accompanied the payment of additional search fees.

It is desirable to stabilize the C-domain in order to increase the calcium stability and/or thermostability of the enzyme. In this connection the stabilization may result in a stabilization of the binding of calcium by the enzyme, and an improved
5 contact between the C-domain and the A-domain (of importance for thermostability). The latter may be achieved by introduction of cystein bridges, salt bridges or increase hydrogen, hydrophobic and/or electrostatic interactions.

10 For instance, the C-domain of the *B. licheniformis* α -amylase having the amino acid sequence shown in SEQ ID No. 2 may be stabilized by introduction of a cystein bridge between domain A and domain C, e.g. by introducing of the following mutations: A349C+I479C and/or L346C+I430C.

15

A salt bridge may be obtained by introduction of the following mutations:

N457D,E

N457D,E+K385R

20 F350D,E+I430R,K

F350D,E+I411R,K

The calcium site of Domain C may be stabilized by replacing the amino acid residues H408 and/or G303 with any other amino acid
25 residue. Of particular interest is the following mutations:

H408Q,E,N,D and/or G303N,D,Q,E

which are contemplated to provide a better calcium binding or protection from calcium depletion.

30 Similar mutations may be introduced in equivalent positions of other Termamyl-like α -amylases.

Other substitution mutations (relative to *B. licheniformis* α -amylase, SEQ ID No. 2) which appear to be of importance,
35 *inter alia*, in the context of reducing calcium dependency include the following: R23K, H156Y, A181T, A209V and G310D (or equivalent mutations in equivalent positions in another Termamyl-like α -amylase). Substitutions of R214 and P345 with

other amino acids may also be of importancen in this connection.

Variants with altered activity at higher/lower pH

5

It is contemplated that it is possible to change the pH optima of a Termamyl-like α -amylase or the enzymatic activity at a given pH by changing the pKa of the active site residues. This may be achieved, e.g. by changing the electrostatic interaction
10 or hydrophobic interaction between functional groups of amino acid side chains of the amino acid residue to be modified and of its close surroundings. This may, e.g., be accomplished by the following method:

15 i) in a structure of the Termamyl-like α -amylase in question to identifying an amino acid residue within 15Å from an active site residue, in particuluar 10Å from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site
20 residue,

ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and
25 evaluating the accomodation of the amino acid residue in the structure,

iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into
30 the structure,

iv) constructing a Termamyl-like α -amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent enzymatic activity of interest of said variant.

35

In the above method it may be of particular relevance to add a positively charged residue within 5Å of a glutamate (thereby lowering the pKa of the glutamate from about 4.5 to 4), or to

add a negatively charged residue within 5 Å of a glutamate (thereby increasing the pKa to about 5), or to make similar modifications within a distance of about 5Å of a Histidine.

5 In a further aspect the invention relates to a variant of a Termamyl-like α -amylase which exhibits a higher activity at a lower pH (e.g. compared to the pH optimum) than the parent α -amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the
10 following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

E336, Q333, P331, I236, V102, A232, I103, L196

The following mutations are of particular interest:

15

E336R, K

Q333R, K

P331R, K

V102R, K, A, T, S, G;

20 I236K, R, N;

I103K, R;

L196K, R;

A232T, S, G;

25 or any combination of two or more of these variants or any combination of one or more of these variants with any of the other variants disclosed herein.

In a still further aspect the invention relates to a variant of
30 a Termamyl-like α -amylase which has a higher activity at a higher pH than the parent α -amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

35

N236, H281, Y273

In particular, the variant comprises a mutation corresponding to at least one of the following mutations of the *B. licheniformis* α -amylase (SEQ ID NO 2):

5 N326I,Y,F,L,V
H281F,I,L
Y273F,W

or any combination of two or more of these variants or any
10 combination of one or more of these variants with any of the other variants disclosed herein.

A mutation which appears to be importance in relation to the specific activity of variants of the invention is a mutation
15 corresponding to the substitution S187D in *B. licheniformis* α -amylase (SEQ ID NO 2).

Variants with increased thermostability and/or altered temperature optimum

20

In a further desired aspect the invention relates to a variant of a parent Termamyl-like α -amylase, which variant is the result of one or more amino acid residues having been deleted from, replaced or added to the parent α -amylase so as to obtain
25 an increased thermostability of the variant.

The Termamyl-like α -amylase structure contains a number of unique internal holes, which may contain water, and a number of crevices. In order to increase the thermostability of the α -
30 amylase it may be desirable to reduce the number of holes and crevices (or reduce the size of the holes or crevices), e.g. by introducing one or more hydrophobic contacts, preferably achieved by introducing bulkier residues, in the vicinity or surroundings of the hole. For instance, the amino acid residues
35 to be modified are those which are involved in the formation of the hole.

Accordingly, in a further aspect the present invention relates to a method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α -amylase, which method comprises

- 5 i) identifying an internal hole or a crevice of the parent Termamyl-like α -amylase in the three-dimensional structure of said α -amylase,
- 10 ii) replacing, in the structure, one or more amino acid residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of
- 15 the hole or crevice,
- iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.
- 20 The structure used for identifying the hole or crevice of the parent Termamyl-like α -amylase may be the structure identified in Appendix 1 or a model structure of the parent Termamyl-like α -amylase built thereon.
- 25 It will be understood that the hole or crevice is identified by the amino acid residues surrounding the hole/crevice, and that modification of said amino acid residues are of importance for filling or reducing the size of the hole/crevice. The particular amino acid residues referred to below are those
- 30 which in crystal structure have been found to flank the hole/crevice in question.

In order to fill (completely or partly) a major hole located between domain A and B, mutation to any other amino acid

35 residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143,
R146

5

Of particular interest is a mutation to a more bulky amino acid residue than the amino acid residue of the parent enzyme.

Of particular interest is a variant of a Termamyl-like α -
10 amylase which comprises a mutation corresponding to the following mutations (using the numbering of *B. licheniformis* α -amylase (SEQ ID NO 2):

L61W, V, F;
15 Y62W;
F67W;
K106R, F, W;
G145F, W
I212F, L, W, Y, R, K;
20 S151 replaced with any other amino acid residue and in particular with F, W, I or L;
R214W;
Y150R, K;
F143W; and/or
25 R146W.

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues
30 of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L241, I236.

35 Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

5 L241I,F,Y,W; and/or
I236L,F,W,Y

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid
10 residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L7, V259, F284

15 Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

20

L7F,I,W
V259F,I,L
F284W

25 In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

30

F350, F343

Of interest is a mutation to a more bulky amino acid residue.

35 Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:
F350W

F343W

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) is contemplated:

L427, V481

10

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α -amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α -amylase:

L427F,L,W

V481,F,I,L,W

20 Variants with an altered cleavage pattern

In the starch liquefaction process it is desirable to use an α -amylase which is capable of degrading the starch molecules into long branched oligo saccharides (like, e.g. the Fungamyl-like α -amylases) rather than shorter branched oligo saccharides (like conventional Termamyl-like α -amylases). The resulting very small branched oligosaccharides (panose precursors) cannot be hydrolyzed properly by pullulanases, which in the liquefaction process are used after the α -amylases and before the amyloglucosidases. Thus, in the presence of panose precursors the action of amylo-glucoamylase ends up with a high degree of the small branched limiting-dextrin, the trisaccharide panose. The presence of panose lowers the saccharification yield significantly and is thus undesirable.

35 Thus, one aim of the present invention is to change the degradation characteristics of a Termamyl-like α -amylase to that of a Fungamyl-like α -amylases without at the same time reducing the thermostability of the Termamyl-like α -amylase.

Accordingly, in a further aspect the invention relates to a variant of a Termamyl-like α -amylase which has a reduced ability to cleave a substrate close to the branching point.

5 The variant may suitably be constructed by a method which comprises

i) identifying the substrate binding area of the parent Termamyl-like α -amylase in a model of the three-dimensional
10 structure of said α -amylase, (e.g. within a sphere of 4Å from the substrate binding site (as defined in the section above entitled "Substrate Binding Site"),

ii) replacing, in the model, one or more amino acid residues of
15 the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of the parent α -amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more
20 amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and

25 iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

Of particular interest is a variant which cleaves an
30 amylopectin substrate, from the reducing end, more than one glucose unit from the branching point, preferably more than two or three glucose units from the branching point, i.e. at a further distance from the branching point than that obtained by use of a wild type *B. licheniformis* α -amylase.

35

Residues of particular interest in connection with this aspect of the invention correspond to the following residues of the *B. licheniformis* α -amylase (SEQ ID NO 2): V54, D53, Y56, Q333,

G57, and the variants according to this aspect preferably comprises a mutation in one or more of these residues.

In particular, the variant comprises at least one of the following mutations, which are expected to prevent cleavage close to the branching point:

V54L, I, F, Y, W, R, K, H, E, Q

D53L, I, F, Y, W

10 Y56W

Q333W

G57all possible amino acid residues

A52amino acid residues larger than A, e.g. A52W, Y, L, F, I.

15 Variants of a fungal α -amylase

In a still further embodiment the invention relates to a variant of a parent Fungamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α -amylase as a template.

30

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α -amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 10, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 4, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 10,

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

A specific example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

Another example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 4.

In a further embodiment the invention relates to a variant of a parent Fungamyl-like α -amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the amino acid sequence shown in SEQ ID No. 10 has been deleted.

General mutations in variants of the invention

It may be preferred that the variant of the invention or prepared in accordance with the method of the invention comprises one or more modifications in addition to those outlined above. Thus, it may be advantageous that one or more proline residues present in the part of the α -amylase variant

having been modified is/are replaced with a non-proline residue which may be any of the possible, naturally occurring non-proline residues, and which preferably is an alanine, glycine, serine, threonine, valine or leucine.

5

Analogously, it may be preferred that one or more cysteine residues present in the amino acid residues with which the parent α -amylase is modified are replaced with a non-cysteine residues such as serine, alanine, threonine, glycine, valine or
10 leucine.

Furthermore, the variant of the invention may either as the only modification or in combination with any of the above outlined modifications be modified so that one or more Asp
15 and/or Glu present in an amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively. Also of interest is the modification of one or more of the Lys residues present in the Termamyl-like α -amylase is replaced by an Arg present in an
20 amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively.

It will be understood that in accordance with the present
25 invention variants may be prepared which carry two or more of the above outlined modifications. For instance, variants may be prepared which comprises a modification in the loop 1 and loop 2 region, a modification in loop 2 and limited loop 3, a modification in loop 1, loop 2, loop 3 and loop 8, etc.

30

Furthermore, it may be advantageous to introduce point-mutations in any of the variants described herein.

Methods of preparing α -amylase variants

35 Several methods for introducing mutations into genes are known in the art. After a brief discussion of the cloning of α -amylase-encoding DNA sequences, methods for generating

mutations at specific sites within the α -amylase-encoding sequence will be discussed.

Cloning a DNA sequence encoding an α -amylase

- 5 The DNA sequence encoding a parent α -amylase may be isolated from any cell or microorganism producing the α -amylase in question, using various methods well known in the art. First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that pro-
- 10 duces the α -amylase to be studied. Then, if the amino acid sequence of the α -amylase is known, homologous, labelled oligonucleotide probes may be synthesized and used to identify α -amylase-encoding clones from a genomic library prepared from the organism in question. Alternatively, a labelled oligonu-
- 15 cleotide probe containing sequences homologous to a known α -amylase gene could be used as a probe to identify α -amylase-encoding clones, using hybridization and washing conditions of lower stringency.
- 20 Yet another method for identifying α -amylase-encoding clones would involve inserting fragments of genomic DNA into an expression vector, such as a plasmid, transforming α -amylase-negative bacteria with the resulting genomic DNA library, and then plating the transformed bacteria onto agar containing a
- 25 substrate for α -amylase, thereby allowing clones expressing the α -amylase to be identified.

Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g.

30 the phosphoroamidite method described by S.L. Beaucage and M.H. Caruthers (1981) or the method described by Matthes et al. (1984). In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned in appropriate vectors.

35

Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by ligating fragments of synthetic,

genomic or cDNA origin (as appropriate, the fragments corresponding to various parts of the entire DNA sequence), in accordance with standard techniques. The DNA sequence may also be prepared by polymerase chain reaction (PCR) using specific
5 primers, for instance as described in US 4,683,202 or R.K. Saiki et al. (1988).

Site-directed mutagenesis

Once an α -amylase-encoding DNA sequence has been isolated, and
10 desirable sites for mutation identified, mutations may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites; mutant nucleotides are inserted during oligonucleotide synthesis. In a specific method, a single-stranded
15 gap of DNA, bridging the α -amylase-encoding sequence, is created in a vector carrying the α -amylase gene. Then the synthetic nucleotide, bearing the desired mutation, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment)
20 and the construct is ligated using T4 ligase. A specific example of this method is described in Morinaga et al. (1984). US 4,760,025 discloses the introduction of oligonucleotides encoding multiple mutations by performing minor alterations of the cassette. However, an even greater variety of mutations can
25 be introduced at any one time by the Morinaga method, because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method of introducing mutations into α -amylase-encoding
30 DNA sequences is described in Nelson and Long (1989). It involves the 3-step generation of a PCR fragment containing the desired mutation introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment carrying the mutation
35 may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

Random mutagenesis

Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

5

For region-specific random mutagenesis with a view to improving the thermal stability of a parent Termamyl-like α -amylase, codon positions corresponding to the following amino acid residues of the *B. licheniformis* α -amylase (SEQ ID NO 2) may
10 appropriately be targeted:

To improve the stability of the calcium site between Domain A and C

I428-A435

15 T297-L308

F403-V409

To improve the stability between domain A and B:

D180-D204

20 H156-T163

A232-F238

With a view to achieving improved binding of a substrate (i.e. improved binding of a carbohydrate species, such as amylose or
25 amylopectin) by a Termamyl-like α -amylase variant, modified (e.g. higher) substrate specificity and/or modified (e.g. higher) specificity with respect to cleavage (hydrolysis) of substrate, it appears that the following codon positions for the amino acid sequence shown in SEQ ID NO 2 (or equivalent
30 codon positions for another parent Termamyl-like α -amylase in the context of the invention) may particularly appropriately be targeted:

13-18

35 50-56

70-76

102-109

163-172

189-199

229-235

360-264

327-335

5

The random mutagenesis of a DNA sequence encoding a parent α -amylase to be performed in accordance with step a) of the above-described method of the invention may conveniently be performed by use of any method known in the art.

10

For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents.

The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues.

When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

35

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleo-

5 tide at the positions which are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the amylolytic enzyme by any published technique, using e.g. PCR, LCR or any DNA polymerase and ligase.

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent α -amylase enzyme
10 is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., Technique, Vol.1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., Molec. Gen. Genet.,
15 133, 1974, pp. 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the amylolytic enzyme by e.g. transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated
20 plasmid from the mutator strain. The mutated plasmid may subsequently be transformed into the expression organism.

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent amylolytic enzyme. Alternatively, the DNA
25 sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenizing agent. The DNA to be mutagenized may also be present in a host cell either by being
30 integrated in the genome of said cell or by being present on a vector harboured in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

35

In some cases it may be convenient to amplify the mutated DNA sequence prior to the expression step (b) or the screening step (c) being performed. Such amplification may be performed in

accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

5 Subsequent to the incubation with or exposure to the mutagenizing agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this
10 purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: grampositive bacteria such as *Bacillus subtilis*,
15 *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gramnegative
20 bacteria such as *E.coli*.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

25 Localized random mutagenesis: the random mutagenesis may advantageously be localized to a part of the parent α -amylase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular
30 importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

35 The localized random mutagenesis is conveniently performed by use of PCR-generated mutagenesis techniques as described above or any other suitable technique known in the art.

Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g. by being inserted into a suitable vector, and said part may subsequently be subjected to mutagenesis by use of any of the mutagenesis methods
5 discussed above.

With respect to the screening step in the above-mentioned method of the invention, this may conveniently be performed by use of a filter assay based on the following principle:

10

A microorganism capable of expressing the mutated amylolytic enzyme of interest is incubated on a suitable medium and under suitable conditions for the enzyme to be secreted, the medium being provided with a double filter comprising a first protein-
15 binding filter and on top of that a second filter exhibiting a low protein binding capability. The microorganism is located on the second filter. Subsequent to the incubation, the first filter comprising enzymes secreted from the microorganisms is separated from the second filter comprising the microorganisms.
20 The first filter is subjected to screening for the desired enzymatic activity and the corresponding microbial colonies present on the second filter are identified.

The filter used for binding the enzymatic activity may be any
25 protein binding filter e.g. nylon or nitrocellulose. The top-filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins e.g. cellulose acetate or Durapore™. The filter may be pretreated with any of the conditions to be used for screening
30 or may be treated during the detection of enzymatic activity.

The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any other known technique for detection of enzymatic activity.

35

The detecting compound may be immobilized by any immobilizing agent e.g. agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents.

α -Amylase activity is detected by Cibacron Red labelled amylopectin, which is immobilized on agarose. For screening for variants with increased thermal and high-pH stability, the filter with bound α -amylase variants is incubated in a buffer
5 at pH 10.5 and 60° or 65°C for a specified time, rinsed briefly in deionized water and placed on the amylopectin-agarose matrix for activity detection. Residual activity is seen as lysis of Cibacron Red by amylopectin degradation. The conditions are chosen to be such that activity due to the α -amylase having the
10 amino acid sequence shown in SEQ ID No.1 can barely be detected. Stabilized variants show, under the same conditions, increased colour intensity due to increased liberation of Cibacron Red.

15 For screening for variants with an activity optimum at a lower temperature and/or over a broader temperature range, the filter with bound variants is placed directly on the amylopectin-Cibacron Red substrate plate and incubated at the desired temperature (e.g. 4°C, 10°C or 30°C) for a specified time.
20 After this time activity due to the α -amylase having the amino acid sequence shown in SEQ ID No.1 can barely be detected, whereas variants with optimum activity at a lower temperature will show increase amylopectin lysis. Prior to incubation onto the amylopectin matrix, incubation in all kinds of desired
25 media - e.g. solutions containing Ca^{2+} , detergents, EDTA or other relevant additives - can be carried out in order to screen for changed dependency or for reaction of the variants in question with such additives.

30

Testing of variants of the invention

The testing of variants of the invention may suitably be performed by determining the starch-degrading activity of the
35 variant, for instance by growing host cells transformed with a DNA sequence encoding a variant on a starch-containing agarose plate and identifying starch-degrading host cells. Further testing as to altered properties (including specific activity,

substrate specificity, cleavage pattern, thermoactivation, pH optimum, pH dependency, temperature optimum, and any other parameter) may be performed in accordance with methods known in the art.

5

Expression of α -amylase variants

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in enzyme form,
10 using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

15 The recombinant expression vector carrying the DNA sequence encoding an α -amylase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector will often depend on the host cell into which it is to be introduced. Thus, the vector
20 may be an autonomously replicating vector, i.e. a vector which exists as an extrachromosomal entity, the replication of which is independent of chromosomal replication, e.g. a plasmid, a bacteriophage or an extrachromosomal element, minichromosome or an artificial chromosome. Alternatively, the vector may be one
25 which, when introduced into a host cell, is integrated into the host cell genome and replicated together with the chromosome(s) into which it has been integrated.

In the vector, the DNA sequence should be operably connected to
30 a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell. Examples of suitable promoters for directing the transcription of the DNA
35 sequence encoding an α -amylase variant of the invention, especially in a bacterial host, are the promoter of the *lac* operon of *E. coli*, the *Streptomyces coelicolor* agarase gene *dagA* promoters, the promoters of the *Bacillus licheniformis* α -

amylase gene (*amyL*), the promoters of the *Bacillus stearothermophilus* maltogenic amylase gene (*amyM*), the promoters of the *Bacillus amyloliquefaciens* α -amylase (*amyQ*), the promoters of the *Bacillus subtilis* *xylA* and *xylB* genes etc. For
5 transcription in a fungal host, examples of useful promoters are those derived from the gene encoding *A. oryzae* TAKA amylase, *Rhizomucor miehei* aspartic proteinase, *A. niger* neutral α -amylase, *A. niger* acid stable α -amylase, *A. niger* glucoamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline
10 protease, *A. oryzae* triose phosphate isomerase or *A. nidulans* acetamidase.

The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, poly-
15 adenylation sequences operably connected to the DNA sequence encoding the α -amylase variant of the invention. Termination and polyadenylation sequences may suitably be derived from the same sources as the promoter.

20 The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

25 The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, such as the *dal* genes from *B. subtilis* or *B. licheniformis*, or one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracyclin resistance. Fur-
30 thermore, the vector may comprise *Aspergillus* selection markers such as *amdS*, *argB*, *niaD* and *sC*, a marker giving rise to hygromycin resistance, or the selection may be accomplished by co-transformation, e.g. as described in WO 91/17243.

35 While intracellular expression may be advantageous in some respects, e.g. when using certain bacteria as host cells, it is generally preferred that the expression is extracellular. In general, the *Bacillus* α -amylases mentioned herein comprise a

preregion permitting secretion of the expressed protease into the culture medium. If desirable, this preregion may be replaced by a different preregion or signal sequence, conveniently accomplished by substitution of the DNA sequences encoding the respective preregions.

The procedures used to ligate the DNA construct of the invention encoding an α -amylase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of an α -amylase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are grampositive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, or *Streptomyces lividans* or *Streptomyces*

murinus, or gramnegative bacteria such as *E.coli*. The transformation of the bacteria may, for instance, be effected by protoplast transformation or by using competent cells in a manner known *per se*.

5

The yeast organism may favourably be selected from a species of *Saccharomyces* or *Schizosaccharomyces*, e.g. *Saccharomyces cerevisiae*. The filamentous fungus may advantageously belong to a species of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergil-*
10 *lus niger*. Fungal cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells is described in EP 238 023.

15

In a yet further aspect, the present invention relates to a method of producing an α -amylase variant of the invention, which method comprises cultivating a host cell as described above under conditions conducive to the production of the
20 variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and
25 obtaining expression of the α -amylase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

30 The α -amylase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium
35 sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

Industrial Applications

The α -amylase variants of this invention possesses valuable properties allowing for various industrial applications. In particular the enzyme variants finds potential applications as
5 a component in washing, dishwashing and hard surface cleaning detergent compositions, but it may also be useful in the production of sweeteners and ethanol from starch and for textile desizing. Conditions for conventional starch converting processes and liquefaction and/or saccharification processes
10 are described in for instance US Patent No. 3,912,590 and EP patent publications Nos. 252,730 and 63,909.

Production of sweetners from starch: A "traditional" process for conversion of starch to fructose syrups normally consists
15 of three consecutive enzymatic processes, viz. a liquefaction process followed by a saccharification process and an isomerization process. During the liquefaction process, starch is degraded to dextrins by an α -amylase (e.g. Termamyl™) at pH values between 5.5 and 6.2 and at temperatures of 95-160°C for
20 a period of approx. 2h. In order to ensure an optimal enzyme stability under these conditions, 1mM of calcium is added (40 ppm free calcium ions).

After the liquefaction process the dextrins are converted into
25 dextrose by addition of a glucoamylase (e.g. AMG™) and a debranching enzyme, such as an isoamylase or a pullulanase (e.g. Promozyme™). Before this step the pH is reduced to a value below 4.5, maintaining the high temperature (above 95°C), and the liquefying α -amylase activity is denatured. The tem-
30 perature is lowered to 60°C, and glucoamylase and debranching enzyme are added. The saccharification process proceeds for 24-72 hours.

After the saccharification process the pH is increased to a
35 value in the range of 6-8, preferably pH 7.5, and the calcium is removed by ion exchange. The dextrose syrup is then converted into high fructose syrup using, e.g., an immobilized glucoseisomerase (such as Sweetzyme™).

At least 3 enzymatic improvements of this process could be obtained. All three improvements could be seen as individual benefits, but any combination (e.g. 1+2, 1+3, 2+3 or 1+2+3) could be employed:

5

Improvement 1. Reduction of the calcium dependency of the liquefying α -amylase.

Addition of free calcium is required to ensure adequately high
10 stability of the α -amylase, but free calcium strongly inhibits the activity of the glucose isomerase and needs to be removed, by means of an expensive unit operation, to an extent which reduces the level of free calcium to below 3-5 ppm. Cost savings could be obtained if such an operation could be avoided
15 and the liquefaction process could be performed without addition of free calcium ions.

To achieve that, a less calcium-dependent Termamyl-like α -amylase which is stable and highly active at low
20 concentrations of free calcium (< 40 ppm) is required. Such a Termamyl-like α -amylase should have a pH optimum at a pH in the range of 4.5-6.5, preferably in the range of 4.5-5.5.

Improvement 2. Reduction of formation of unwanted Maillard
25 products

The extent of formation of unwanted Maillard products during the liquefaction process is dependent on the pH. Low pH favours reduced formation of Maillard products. It would thus be
30 desirable to be able to lower the process pH from around pH 6.0 to a value around pH 4.5; unfortunately, all commonly known, thermostable Termamyl-like α -amylases are not very stable at low pH (i.e. pH < 6.0) and their specific activity is generally low.

35

Achievement of the above-mentioned goal requires a Termamyl-like α -amylase which is stable at low pH in the range of

4.5-5.5 and at free calcium concentrations in the range of 0-40 ppm, and which maintains a high specific activity.

Improvement 3.

5

It has been reported previously (US patent 5,234,823) that when saccharifying with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase, the presence of residual α -amylase activity from the liquefaction process can lead to lower yields of
10 dextrose if the α -amylase is not inactivated before the saccharification stage. This inactivation can typically be carried out by adjusting the pH to below 4.3 at 95°C, before lowering the temperature to 60°C for saccharification.

15 The reason for this negative effect on dextrose yield is not fully understood, but it is assumed that the liquefying α -amylase (for example Termamyl™ 120 L from *B. licheniformis*) generates "limit dextrins" (which are poor substrates for *B. acidopullulyticus* pullulanase) by hydrolysing 1,4-alpha-
20 glucosidic linkages close to and on both sides of the branching points in amylopectin. Hydrolysis of these limit dextrins by glucoamylase leads to a build-up of the trisaccharide panose, which is only slowly hydrolysed by glucoamylase.

25 The development of a thermostable α -amylase which does not suffer from this disadvantage would be a significant process improvement, as no separate inactivation step would be required.

30 If a Termamyl-like, low-pH-stable α -amylase is developed, an alteration of the specificity could be an advantage needed in combination with increased stability at low pH.

The methodology and principles of the present invention make it
35 possible to design and produce variants according to the invention having the required properties as outlined above.

Detergent Compositions

According to the invention, the α -amylase may typically be a component of a detergent composition. As such, it may be included in the detergent composition in the form of a non-dusting granulate, a stabilized liquid, or a protected enzyme.

5 Non-dusting granulates may be produced, e.g. as disclosed in US 4,106,991 and 4,661,452 (both to Novo Industri A/S) and may optionally be coated by methods known in the art. Examples of waxy coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to

10 20000, ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and mono- and di- and triglycerides of fatty acids. Examples of

15 film-forming coating materials suitable for application by fluid bed techniques are given in patent GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods.

20 Other enzyme stabilizers are well known in the art. Protected enzymes may be prepared according to the method disclosed in EP 238,216.

The detergent composition of the invention may be in any convenient form, e.g. as powder, granules, paste or liquid. A

25 liquid detergent may be aqueous, typically containing up to 70% of water and 0-30% of organic solvent, or nonaqueous.

The detergent composition comprises one or more surfactants, each of which may be anionic, nonionic, cationic, or zwitter-

30 ionic. The detergent will usually contain 0-50% of anionic surfactant such as linear alkylbenzenesulfonate (LAS), alpha-olefinsulfonate (AOS), alkyl sulfate (fatty alcohol sulfate) (AS), alcohol ethoxysulfate (AEOS or AES), secondary alkane-sulfonates (SAS), alpha-sulfo fatty acid methyl esters, alkyl-

35 or alkenylsuccinic acid or soap. It may also contain 0-40% of nonionic surfactant such as alcohol ethoxylate (AEO or AE), carboxylated alcohol ethoxylates, nonylphenol ethoxylate, alkylpolyglycoside, alkyl dimethylamineoxide, ethoxylated fatty

acid monoethanolamide, fatty acid monoethanolamide, or polyhydroxy alkyl fatty acid amide (e.g. as described in WO 92/06154).

- 5 The detergent composition may additionally comprise one or more other enzymes, such as lipase, cutinase, protease, cellulase, peroxidase, e.g., laccase.

The detergent may contain 1-65% of a detergent builder or
10 complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, citrate, nitrilotriacetic acid (NTA), ethylenediaminetetraacetic acid (EDTA), diethylenetriaminepentaacetic acid (DTMPA), alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst). The
15 detergent may also be unbuilt, i.e. essentially free of detergent builder.

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose (CMC), poly(vinylpyrrolidone) (PVP),
20 polyethyleneglycol (PEG), poly(vinyl alcohol) (PVA), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise
25 a H_2O_2 source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetythylenediamine (TAED) or nonanoyloxybenzenesulfonate (NOBS). Alternatively, the bleaching system may comprise peroxy acids of e.g. the amide, imide, or sulfone
30 type.

The enzymes of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g. a polyol such as propylene glycol or glycerol, a sugar or sugar
35 alcohol, lactic acid, boric acid, or a boric acid derivative as e.g. an aromatic borate ester, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, or perfume.

The pH (measured in aqueous solution at use concentration) will usually be neutral or alkaline, e.g. 7-11.

Particular forms of detergent compositions within the scope of the invention include:

1) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

	Linear alkylbenzenesulfonate (calculated as acid)	7	-	12%
20	Alcohol ethoxysulfate (e.g. C ₁₂₋₁₈ alcohol, 1-2 EO) or alkyl sulfate (e.g. C ₁₆₋₁₈)	1	-	4%
	Alcohol ethoxylate (e.g. C ₁₄₋₁₅ alcohol, 7 EO)	5	-	9%
	Sodium carbonate (as Na ₂ CO ₃)	14	-	20%
25	Soluble silicate (as Na ₂ O, 2SiO ₂)	2	-	6%
	Zeolite (as NaAlSiO ₄)	15	-	22%
	Sodium sulfate (as Na ₂ SO ₄)	0	-	6%
	Sodium citrate/citric acid (as C ₆ H ₅ Na ₃ O ₇ /C ₆ H ₈ O ₇)	0	-	15%
30	Sodium perborate (as NaBO ₃ ·H ₂ O)	11	-	18%
	TAED	2	-	6%
	Carboxymethylcellulose	0	-	2%
	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0	-	3%
35	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
	Minor ingredients (e.g. suds suppressors, perfume, optical brightener, photobleach)	0	-	5%

2) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

5	Linear alkylbenzenesulfonate (calculated as acid)	6 - 11%
	Alcohol ethoxysulfate (e.g. C ₁₂₋₁₈ alcohol, 1-2 EO or alkyl sulfate (e.g. C ₁₆₋₁₈))	1 - 3%
10	Alcohol ethoxylate (e.g. C ₁₄₋₁₅ alcohol, 7 EO)	5 - 9%
	Sodium carbonate (as Na ₂ CO ₃)	15 - 21%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	1 - 4%
15	Zeolite (as NaAlSiO ₄)	24 - 34%
	Sodium sulfate (as Na ₂ SO ₄)	4 - 10%
	Sodium citrate/citric acid (as C ₆ H ₅ Na ₃ O ₇ /C ₆ H ₈ O ₇)	0 - 15%
	Carboxymethylcellulose	0 - 2%
20	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1 - 6%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
25	Minor ingredients (e.g. suds suppressors, perfume)	0 - 5%

3) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

30	Linear alkylbenzenesulfonate (calculated as acid)	5 - 9%
	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO)	7 - 14%
35	Soap as fatty acid (e.g. C ₁₆₋₂₂ fatty acid)	1 - 3%
	Sodium carbonate (as Na ₂ CO ₃)	10 - 17%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	3 - 9%
	Zeolite (as NaAlSiO ₄)	23 - 33%
	Sodium sulfate (as Na ₂ SO ₄)	0 - 4%
40	Sodium perborate (as NaBO ₃ ·H ₂ O)	8 - 16%

	TAED	2	-	8%
	Phosphonate (e.g. EDTMPA)	0	-	1%
	Carboxymethylcellulose	0	-	2%
5	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0	-	3%
	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
10	Minor ingredients (e.g. suds suppressors, perfume, optical brightener)	0	-	5%

4) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

15	Linear alkylbenzenesulfonate (calculated as acid)	8	-	12%
	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO)	10	-	25%
20	Sodium carbonate (as Na ₂ CO ₃)	14	-	22%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	1	-	5%
	Zeolite (as NaAlSiO ₄)	25	-	35%
	Sodium sulfate (as Na ₂ SO ₄)	0	-	10%
	Carboxymethylcellulose	0	-	2%
25	Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1	-	3%
	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
30	Minor ingredients (e.g. suds suppressors, perfume)	0	-	5%

5) An aqueous liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	-	21%
35	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO or C ₁₂₋₁₅ alcohol, 5 EO)	12	-	18%
	Soap as fatty acid (e.g. oleic acid)	3	-	13%
40	Alkenylsuccinic acid (C ₁₂₋₁₄)	0	-	13%

	Aminoethanol	8	- 18%
	Citric acid	2	- 8%
	Phosphonate	0	- 3%
	Polymers (e.g. PVP, PEG)	0	- 3%
5	Borate (as B_4O_7)	0	- 2%
	Ethanol	0	- 3%
	Propylene glycol	8	- 14%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
10	Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brightener)	0	- 5%

6) An aqueous structured liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	- 21%
20	Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO, or C_{12-15} alcohol, 5 EO)	3	- 9%
	Soap as fatty acid (e.g. oleic acid)	3	- 10%
	Zeolite (as $NaAlSiO_4$)	14	- 22%
	Potassium citrate	9	- 18%
25	Borate (as B_4O_7)	0	- 2%
	Carboxymethylcellulose	0	- 2%
	Polymers (e.g. PEG, PVP)	0	- 3%
30	Anchoring polymers such as, e.g., lauryl methacrylate/acrylic acid copolymer; molar ratio 25:1; MW 3800	0	- 3%
	Glycerol	0	- 5%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
35	Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brighteners)	0	- 5%

7) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

	Fatty alcohol sulfate	5	- 10%
5	Ethoxylated fatty acid monoethanol- amide	3	- 9%
	Soap as fatty acid	0	- 3%
	Sodium carbonate (as Na_2CO_3)	5	- 10%
	Soluble silicate (as $\text{Na}_2\text{O}, 2\text{SiO}_2$)	1	- 4%
	Zeolite (as NaAlSiO_4)	20	- 40%
10	Sodium sulfate (as Na_2SO_4)	2	- 8%
	Sodium perborate (as $\text{NaBO}_3 \cdot \text{H}_2\text{O}$)	12	- 18%
	TAED	2	- 7%
	Polymers (e.g. maleic/acrylic acid copolymer, PEG)	1	- 5%
15	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. optical brightener, suds suppressors, per- fume)	0	- 5%

8) A detergent composition formulated as a granulate comprising

	Linear alkylbenzenesulfonate (calculated as acid)	8	- 14%
25	Ethoxylated fatty acid monoethanol- amide	5	- 11%
	Soap as fatty acid	0	- 3%
	Sodium carbonate (as Na_2CO_3)	4	- 10%
	Soluble silicate (as $\text{Na}_2\text{O}, 2\text{SiO}_2$)	1	- 4%
	Zeolite (as NaAlSiO_4)	30	- 50%
30	Sodium sulfate (as Na_2SO_4)	3	- 11%
	Sodium citrate (as $\text{C}_6\text{H}_5\text{Na}_3\text{O}_7$)	5	- 12%
	Polymers (e.g. PVP, maleic/acrylic acid copolymer, PEG)	1	- 5%
35	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
	Minor ingredients (e.g. suds suppressors, perfume)	0	- 5%

9) A detergent composition formulated as a granulate comprising

	Linear alkylbenzenesulfonate (calculated as acid)	6	- 12%
	Nonionic surfactant	1	- 4%
5	Soap as fatty acid	2	- 6%
	Sodium carbonate (as Na_2CO_3)	14	- 22%
	Zeolite (as NaAlSiO_4)	18	- 32%
	Sodium sulfate (as Na_2SO_4)	5	- 20%
	Sodium citrate (as $\text{C}_6\text{H}_5\text{Na}_3\text{O}_7$)	3	- 8%
10	Sodium perborate (as $\text{NaBO}_3 \cdot \text{H}_2\text{O}$)	4	- 9%
	Bleach activator (e.g. NOBS or TAED)	1	- 5%
	Carboxymethylcellulose	0	- 2%
15	Polymers (e.g. polycarboxylate or PEG)	1	- 5%
	Enzymes (calculated as pure enzyme protein)	0.0001	- 0.1%
20	Minor ingredients (e.g. optical brightener, perfume)	0	- 5%

10) An aqueous liquid detergent composition comprising

	Linear alkylbenzenesulfonate (calculated as acid)	15	- 23%
25	Alcohol ethoxysulfate (e.g. C_{12-15} alcohol, 2-3 EO)	8	- 15%
	Alcohol ethoxylate (e.g. C_{12-15} al- cohol, 7 EO, or C_{12-15} alcohol, 5 EO)	3	- 9%
30	Soap as fatty acid (e.g. lauric acid)	0	- 3%
	Aminoethanol	1	- 5%
	Sodium citrate	5	- 10%
	Hydrotrope (e.g. sodium toluenesulfonate)	2	- 6%
35	Borate (as B_4O_7)	0	- 2%
	Carboxymethylcellulose	0	- 1%
	Ethanol	1	- 3%
	Propylene glycol	2	- 5%

5	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
	Minor ingredients (e.g. polymers, dispersants, perfume, optical brighteners)	0 - 5%

11) An aqueous liquid detergent composition comprising

10	Linear alkylbenzenesulfonate (calculated as acid)	20 - 32%
	Alcohol ethoxylate (e.g. C ₁₂₋₁₅ alcohol, 7 EO, or C ₁₂₋₁₅ alcohol, 5 EO)	6 - 12%
	Aminoethanol	2 - 6%
	Citric acid	8 - 14%
15	Borate (as B ₄ O ₇)	1 - 3%
20	Polymer (e.g. maleic/acrylic acid copolymer, anchoring polymer such as, e.g., lauryl methacrylate/acrylic acid copolymer)	0 - 3%
	Glycerol	3 - 8%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
25	Minor ingredients (e.g. hydro-tropes, dispersants, perfume, optical brighteners)	0 - 5%

12) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

30	Anionic surfactant (linear alkylbenzenesulfonate, alkyl sulfate, alpha-olefinsulfonate, alpha-sulfo fatty acid methyl esters, alkanesulfonates, soap)	25 - 40%
	Nonionic surfactant (e.g. alcohol ethoxylate)	1 - 10%
35	Sodium carbonate (as Na ₂ CO ₃)	8 - 25%
	Soluble silicates (as Na ₂ O, 2SiO ₂)	5 - 15%
	Sodium sulfate (as Na ₂ SO ₄)	0 - 5%
40	Zeolite (as NaAlSiO ₄)	15 - 28%
	Sodium perborate (as NaBO ₃ ·4H ₂ O)	0 - 20%

	Bleach activator (TAED or NOBS)	0 - 5%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
5	Minor ingredients (e.g. perfume, optical brighteners)	0 - 3%

13) Detergent formulations as described in 1) - 12) wherein all or part of the linear alkylbenzenesulfonate is replaced by (C₁₂-C₁₈) alkyl sulfate.

10

14) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

	(C ₁₂ -C ₁₈) alkyl sulfate	9 - 15%
15	Alcohol ethoxylate	3 - 6%
	Polyhydroxy alkyl fatty acid amide	1 - 5%
	Zeolite (as NaAlSiO ₄)	10 - 20%
	Layered disilicate (e.g. SK56 from Hoechst)	10 - 20%
20	Sodium carbonate (as Na ₂ CO ₃)	3 - 12%
	Soluble silicate (as Na ₂ O, 2SiO ₂)	0 - 6%
	Sodium citrate	4 - 8%
	Sodium percarbonate	13 - 22%
	TAED	3 - 8%
25	Polymers (e.g. polycarboxylates and PVP=	0 - 5%
	Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
30	Minor ingredients (e.g. optical brightener, photo bleach, perfume, suds suppressors)	0 - 5%

15) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

(C ₁₂ -C ₁₈) alkyl sulfate	4 - 8%
Alcohol ethoxylate	11 - 15%

	Soap	1	-	4%
	Zeolite MAP or zeolite A	35	-	45%
	Sodium carbonate (as Na_2CO_3)	2	-	8%
	Soluble silicate (as $\text{Na}_2\text{O}, 2\text{SiO}_2$)	0	-	4%
5	Sodium percarbonate	13	-	22%
	TAED	1	-	8%
	Carboxymethyl cellulose	0	-	3%
	Polymers (e.g. polycarboxylates and PVP)	0	-	3%
10	Enzymes (calculated as pure enzyme protein)	0.0001	-	0.1%
	Minor ingredients (e.g. optical brightener, phosphonate, perfume)	0	-	3%

15 16) Detergent formulations as described in 1) - 15) which contain a stabilized or encapsulated peracid, either as an additional component or as a substitute for already specified bleach systems.

20 17) Detergent compositions as described in 1), 3), 7), 9) and 12) wherein perborate is replaced by percarbonate.

18) Detergent compositions as described in 1), 3), 7), 9), 12), 14) and 15) which additionally contain a manganese catalyst.

25 The manganese catalyst may, e.g., be one of the compounds described in "Efficient manganese catalysts for low-temperature bleaching", Nature 369, 1994, pp. 637-639.

19) Detergent composition formulated as a nonaqueous detergent
30 liquid comprising a liquid nonionic surfactant such as, e.g., linear alkoxylated primary alcohol, a builder system (e.g. phosphate), enzyme and alkali. The detergent may also comprise anionic surfactant and/or a bleach system.

35 The α -amylase variant of the invention may be incorporated in concentrations conventionally employed in detergents. It is at present contemplated that, in the detergent composition of the invention, the α -amylase may be added in an amount correspon-

ding to 0.00001-1 mg (calculated as pure enzyme protein) of α -amylase per liter of wash liquor.

Dishwashing Composition

- 5 The dishwashing detergent composition comprises a surfactant which may be anionic, non-ionic, cationic, amphoteric or a mixture of these types. The detergent will contain 0-90% of non-ionic surfactant such as low- to non-foaming ethoxylated propoxylated straight-chain alcohols.
- 10 The detergent composition may contain detergent builder salts of inorganic and/or organic types. The detergent builders may be subdivided into phosphorus-containing and non-phosphorus-containing types. The detergent composition usually contains 1-90% of detergent builders.
- 15 Examples of phosphorus-containing inorganic alkaline detergent builders, when present, include the water-soluble salts especially alkali metal pyrophosphates, orthophosphates, and polyphosphates. An example of phosphorus-containing organic alkaline detergent builder, when present, includes the water-
20 soluble salts of phosphonates. Examples of non-phosphorus-containing inorganic builders, when present, include water-soluble alkali metal carbonates, borates and silicates as well as the various types of water-insoluble crystalline or amorphous alumino silicates of which zeolites are the best-known
25 representatives.

Examples of suitable organic builders include the alkali metal, ammonium and substituted ammonium, citrates, succinates, malonates, fatty acid sulphonates, carboxymethoxy succinates,
30 ammonium polyacetates, carboxylates, polycarboxylates, amino-polycarboxylates, polyacetyl carboxylates and polyhydroxysulphonates.

Other suitable organic builders include the higher molecular
35 weight polymers and co-polymers known to have builder properties, for example appropriate polyacrylic acid, polymaleic and polyacrylic/polymaleic acid copolymers and their salts.

The dishwashing detergent composition may contain bleaching agents of the chlorine/bromine-type or the oxygen-type. Examples of inorganic chlorine/bromine-type bleaches are lithium, sodium or calcium hypochlorite and hypobromite as well
5 as chlorinated trisodium phosphate. Examples of organic chlorine/bromine-type bleaches are heterocyclic N-bromo and N-chloro imides such as trichloroisocyanuric, tribromoisocyanuric, dibromoisocyanuric and dichloroisocyanuric acids, and salts thereof with water-solubilizing cations such as potassium
10 and sodium. Hydantoin compounds are also suitable.

The oxygen bleaches are preferred, for example in the form of an inorganic persalt, preferably with a bleach precursor or as a peroxy acid compound. Typical examples of suitable peroxy
15 bleach compounds are alkali metal perborates, both tetrahydrates and monohydrates, alkali metal percarbonates, persilicates and perphosphates. Preferred activator materials are TAED and glycerol triacetate.

20 The dishwashing detergent composition of the invention may be stabilized using conventional stabilizing agents for the enzyme(s), e.g. a polyol such as e.g. propylene glycol, a sugar or a sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g. an aromatic borate ester.

25

The dishwashing detergent composition of the invention may also contain other conventional detergent ingredients, e.g. deflocculant material, filler material, foam depressors, anti-corrosion agents, soil-suspending agents, sequestering agents,
30 anti-soil redeposition agents, dehydrating agents, dyes, bactericides, fluorescers, thickeners and perfumes.

Finally, the α -amylase variant of the invention may be used in conventional dishwashing detergents, e.g. in any of the
35 detergents described in any of the following patent publications:

EP 518719, EP 518720, EP 518721, EP 516553, EP 516554,

EP 516555, GB 2200132, DE 3741617, DE 3727911, DE 4212166,
DE 4137470, DE 3833047, WO 93/17089, DE 4205071, WO 52/09680,
WO 93/18129, WO 93/04153, WO 92/06157, WO 92/08777, EP 429124,
WO 93/21299, US 5141664, EP 561452, EP 561446, GB 2234980,
5 WO 93/03129, EP 481547, EP 530870, EP 533239, EP 554943,
EP 346137, US 5112518, EP 318204, EP 318279, EP 271155,
EP 271156, EP 346136, GB 2228945, CA 2006687, WO 93/25651,
EP 530635, EP 414197, US 5240632.

10 EXAMPLES

EXAMPLE 1

15 Example on Homology building of TERM

The overall homology of the *B. licheniformis* α -amylase (in the following referred to as TERM) to other Termamyl-like α -amylases is high and the percent similarity is extremely high.
20 The similarity calculated for TERM to BSG (the *B. stearothermophilus* α -amylase with SEQ ID NO 6), and BAN (the *B. amyloliquefaciens* α -amylase with SEQ ID NO 4) using the University of Wisconsin Genetics Computer Group's program GCG gave 89% and 78%, respectively. TERM has a deletion of 2
25 residues between residue G180 and K181 compared to BAN and BSG. BSG has a deletion of 3 residues between G371 and I372 in comparison with BAN and TERM. Further BSG has a C-terminal extension of more than 20 residues compared to BAN and TERM. BAN has 2 residues less and TERM has one residue less in the
30 N-terminal compared to BSG.

The structure of the *B. licheniformis* (TERM) and of the *B. amyloliquefaciens* α -amylase (BAN), respectively, was model built on the structure disclosed in Appendix 1 herein. The
35 structure of other Termamyl-like α -amylases (e.g. those disclosed herein) may be built analogously.

In comparison with the α -amylase used for elucidating the present structure, TERM differs in that it lacks two residues around 178-182. In order to compensate for this in the model structure, the HOMOLOGY program from BIOSYM was used to substitute the residues in equivalent positions in the structure (not only structurally conserved regions) except for the deletion point. A peptide bond was established between G179(G177) and K180(K180) in TERM(BAN). The close structural relationship between the solved structure and the model structure (and thus the validity of the latter) is indicated by the presence of only very few atoms found to be too close together in the model.

To this very rough structure of TERM was then added all waters (605) and ions (4 Calcium and 1 Sodium) from the solved structure (Appendix 1) at the same coordinates as for said solved structure using the INSIGHT program. This could be done with only few overlaps - in other words with a very nice fit. This model structure were then minimized using 200 steps of Steepest descent and 600 steps of Conjugated gradient (see Brooks et al 1983, J. Computational Chemistry 4, p.187-217). The minimized structure was then subjected to molecular dynamics, 5ps heating followed by up to 200ps equilibration but more than 35ps. The dynamics as run with the Verlet algorithm and the equilibration temperature 300K were kept using the Berendsen coupling to a waterbath (Berendsen et. al., 1984, J. Chemical Physics 81, p. 3684-3690). Rotations and translations were removed every picosecond. The potential energy became stable after appr. 35ps equilibration. A mean dynamics structure was extracted and can be used for further analysis.

EXAMPLE 2

Determination of residues within 10Å from the ions present in the solved structure

The coordinates of Appendix 1 are read into the INSIGHT program provided by BIOSYM technologies. The spatial coordinates are

presented showing the bonds between the atoms. The ions are presented as well as the water atoms. The program package part of creating subset are used to create a 10Å subset around the Calcium and the Sodium ions in the structure using the command
5 ZONE. All residues having an atom within the 10Å are compiled and written out by the LIST MOLECULE command. By giving the ions the name ium in the coordinate file a 10Å sphere around all atoms called ium is compiled. The specific residues identified in this manner are given further above in the
10 section entitled "Ca²⁺ dependency".

EXAMPLE 3

Determination of cavities in the solved structure (Appendix 1)

15

The solved structure exhibits many internal holes and cavities. When analysing for such cavities the Connolly program is normally used (Lee, B. and Richards, F.M. (1971) J. Mol. Biol. 55,p. 379-400). The program uses a probe with radius to search
20 the external and internal surface of the protein. The smallest hole observable in this way has the probe radius.

To analyse the solved structure a modified version of the Connolly program included in the program of INSIGHT were used.
25 First the water molecules and the ions were removed by unmerging these atoms from the solved structure. By using the command MOLECULE SURFACE SOLVENT the solvent accessible surface area were calculated for all atoms and residues using a probe radius of 1.4Å, and displayed on the graphics screen together
30 with the model of the solved structure. The internal cavities where then seen as dot surfaces with no connections to external surface.

Mutant suggestions for filling out the holes are given in the
35 specification (in the section entitled "Variants with increased thermostability and/or altered temperature optimum"). By using the homology build structures or/and the sequence alignment

mutations for the homologous structures of TERM and BSG and BAN can be made.

EXAMPLE 4

5

Construction of Termamyl™ variants in accordance with the invention

Termamyl (SEQ ID NO. 2) is expressed in *B. subtilis* from a
10 plasmid denoted pDN1528. This plasmid contains the complete
gene encoding Termamyl, *amyL*, the expression of which is
directed by its own promoter. Further, the plasmid contains the
origin of replication, *ori*, from plasmid pUB110 and the *cat*
gene from plasmid pC194 conferring resistance towards
15 chloramphenicol. pDN1528 is shown in Fig. 9.

A specific mutagenesis vector containing a major part of the
coding region of SEQ ID NO 1 was prepared. The important
features of this vector, denoted pJeEN1, include an origin of
20 replication derived from the pUC plasmids, the *cat* gene
conferring resistance towards chloramphenicol, and a
frameshift-containing version of the *bla* gene, the wild type of
which normally confers resistance towards ampicillin (*amp*^R
phenotype). This mutated version results in an *amp*^S phenotype.
25 The plasmid pJeEN1 is shown in Fig. 10, and the *E. coli* origin
of replication, *ori*, *bla*, *cat*, the 5'-truncated version of the
Termamyl amylase gene, and selected restriction sites are
indicated on the plasmid.

30 Mutations are introduced in *amyL* by the method described by
Deng and Nickoloff (1992, Anal. Biochem. 200, pp. 81-88) except
that plasmids with the "selection primer" (primer #6616; see
below) incorporated are selected based on the *amp*^R phenotype of
transformed *E. coli* cells harboring a plasmid with a repaired
35 *bla* gene, instead of employing the selection by restriction
enzyme digestion outlined by Deng and Nickoloff. Chemicals and
enzymes used for the mutagenesis were obtained from the

Chameleon™ mutagenesis kit from Stratagene (catalogue number 200509).

After verification of the DNA sequence in variant plasmids, the truncated gene, containing the desired alteration, is subcloned into pDN1528 as a *Pst*I-*Eco*RI fragment and transformed into a protease- and amylase-depleted *Bacillus subtilis* strain in order to express the variant enzyme.

- 10 The Termamyl variant V54W was constructed by the use of the following mutagenesis primer (written 5' to 3', left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CGC TTG

- 15 The Termamyl variant A52W + V54W was constructed by the use of the following mutagenesis primer (written 5' to 3', left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CCA TTG GCT CG

20

Primer #6616 (written 5' to 3', left to right; P denotes a 5' phosphate):

P CTG TGA CTG GTG AGT ACT CAA CCA AGT C

25

EXAMPLE 5

Saccharification in the presence of "residual" α -amylase activity

30

Two appropriate Termamyl variants with altered specificity were evaluated by saccharifying a DE 10 (DE = dextrose equivalent) maltodextrin substrate with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase under conditions where the variant amylase was active.

Saccharification: Substrates for saccharification were prepared by dissolving 230 g DE 10 spray-dried maltodextrin, prepared

from common corn starch, in 460 ml boiling deionized water and adjusting the dry substance (DS) content to approximately 30% w/w. The pH was adjusted to 4.7 (measured at 60°C) and aliquots of substrate corresponding to 15 g dry weight were transferred to 50 ml blue cap glass flasks.

The flasks were then placed in a shaking water bath equilibrated at 60°C, and the enzymes added. The pH was readjusted to 4.7 where necessary.

10

The following enzymes were used:

Glucoamylase: AMG™ (Novo Nordisk A/S); dosage 0.18 AG/g DS

Pullulanase: Promozyme™ (Novo Nordisk A/S);

15

dosage 0.06 PUN/g DS

α-Amylases: Termamyl™ (Novo Nordisk A/S); dosage 60 NU/g DS

Termamyl variant V54W; dosage 60 NU/g DS

Termamyl variant V54W + A52W; dosage 60 NU/g DS

20 2 ml samples were taken periodically. The pH of each sample was adjusted to about 3.0, and the sample was then heated in a boiling water bath for 15 minutes to inactivate the enzymes. After cooling, the samples were treated with approximately 0.1 g mixed-bed ion exchange resin (BIO-Rad 501-X (D)) for 30 minutes on a rotary mixer and then filtered. The carbohydrate composition of each sample was determined by HPLC. The following results were obtained after 72 hours [DP_n denotes a dextrose (D-glucose) oligomer with n glucose units]:

30

α-amylase	%DP ₁	%DP ₂	%DP ₃	%DP ₄
None (control)	95.9	2.8	0.4	1.0
V54W	96.0	2.9	0.4	0.8
35 V54W + A52W	95.9	2.8	0.4	0.8
Termamyl™	95.6	2.8	0.8	0.8

It can be seen from the above results that compared with the control (no α -amylase activity present during liquefaction), the presence of α -amylase activity from variants V54W and V54W + A52W did not lead to elevated panose (DP₃) levels. In contrast, Termamyl α -amylase activity resulted in higher levels of panose and a subsequent loss of D-glucose (DP₁) yield.

Thus, if α -amylase variants V54W or V54W + A52W are used for starch liquefaction, it will not be necessary to inactivate the residual α -amylase activity before the commencement of saccharification.

EXAMPLE 6

15 Calcium-binding affinity of α -amylase variants of the invention

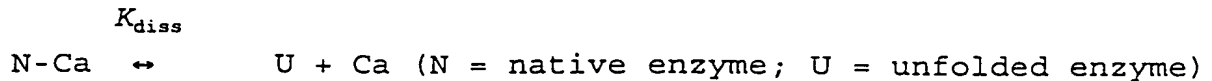
Unfolding of amylases by exposure to heat or to denaturants such as guanidine hydrochloride is accompanied by a decrease in fluorescence. Loss of calcium ions leads to unfolding, and the affinity of α -amylases for calcium can be measured by fluorescence measurements before and after incubation of each α -amylase (e.g. at a concentration of 10 μ g/ml) in a buffer (e.g. 50 mM HEPES, pH 7) with different concentrations of calcium (e.g. in the range of 1 μ M-100 mM) or of EGTA (e.g. in the range of 1-1000 μ M) [EGTA = 1,2-di(2-aminoethoxy)ethane-N,N,N',N'-tetraacetic acid] for a sufficiently long period of time (such as 22 hours at 55°C).

The measured fluorescence F is composed of contributions from the folded and unfolded forms of the enzyme. The following equation can be derived to describe the dependence of F on calcium concentration ($[Ca]$):

$$F = [Ca] / (K_{diss} + [Ca]) (\alpha_N - \beta_N \log([Ca])) + K_{diss} / (K_{diss} + [Ca]) (\alpha_U - \beta_U \log([Ca]))$$

where α_N is the fluorescence of the native (folded) form of the enzyme, β_N is the linear dependence of α_N on the logarithm of

the calcium concentration (as observed experimentally), α_u is the fluorescence of the unfolded form and β_u is the linear dependence of α_u on the logarithm of the calcium concentration. K_{diss} is the apparent calcium-binding constant for an equilibrium process as follows:



10 In fact, unfolding proceeds extremely slowly and is irreversible. The rate of unfolding is dependent on calcium concentration, and the dependency for a given α -amylase provides a measure of the Ca-binding affinity of the enzyme. By defining a standard set of reaction conditions (e.g. 22 hours
15 at 55°C), a meaningful comparison of K_{diss} for different α -amylases can be made. The calcium dissociation curves for α -amylases in general can be fitted to the equation above, allowing determination of the corresponding values of K_{diss} .

20 The following values for K_{diss} were obtained for a parent Termamyl-like α -amylase having the amino acid sequence shown in SEQ ID No. 1 of WO 95/26397 and for the indicated variant thereof according to the invention:

25 α -Amylase	K_{diss} (mol/l)
L351C + M430C + T183* + G184*	$1.7 (\pm 0.5) \times 10^{-3}$
Parent	$3.5 (\pm 1.1) \times 10^{-1}$

30

It is apparent from the above that the calcium-binding affinity of the variant in question binds calcium significantly more strongly than the parent, and thereby has a correspondingly lower calcium dependency than the parent.

35

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SEQUENCE LISTING

In the following SEQ ID Nos. 1, 3, 5 the 5', coding sequence and 3' sequence of the relevant α -amylase genes are illustrated. The 5' sequence is the first separate part of the sequence written with lower case letters, the coding sequence is the intermediate part of the sequence, where the signal sequence is written with lower case letters and the sequence encoding the mature α -amylase is written with upper case letters, and the 3' sequence is the third separate part of the sequence written with lower case letters.

SEQ ID No. 1

15
cggaagattggaagtacaaaaataagcaaaagattgtcaatcatgtcatgagccatgcgg-
gagacggaaaaatcgtctta atgcacgatattttatgcaacgttcgcagatgctgctgaa-
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15 SEQ ID No. 2

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DYFDH HDIVGWTREGDSSVANSGLAALITDGP GGAKRMYV
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VQR

30

SEQ ID No. 3

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SEQ ID No. 4

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5 LQDAIGSLHSRNVQVYGDVVLN HKAGADATEDVTAVEVNP
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15

SEQ ID No. 5

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15

SEQ ID No. 6

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30 GKQHAGKVFYDLTGNRSDTVTINSDGWGEFKVNGGSVSVW
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SEQ ID No. 10

35 1 ATPADWRSQS IYFLLTDRFA RTDGSTTATC
31 NTADQKYCGG TWQGIIDKLD YIQGMGFTAI
61 WITPVTALP QTTAYGDAYH GYWQQDIYSL
91 NENYGTADDL KALSSALHER GMYLMVDVVA

121 NHMGYDGAGS SVDYSVFKPF SSQDYFHPFC
151 FIQNYEDQTQ VEDCWLGDNT VSLPDLDTTK
181 DVVKNEWYDW VGSLVSNYSI DGLRIDTVKH
211 VQKDFWPGYN KAAGVYCIGE VLDGDPAYTC
5 241 PYQNVMDGVL NYPIYYPLLN AFKSTSGSMD
271 DLYNMINTVK SDCPDSTLLG TFVENHDNPR
301 FASYTNDIAL AKNVAAFIIL NDGIPIIYAG
331 QEQHYAGGND PANREATWLS GYPTDSELYK
361 LIASANAIRN YAISKDTGFV TYKNWPIYKD
10 391 DITIAMRKGT DGSQIVTILS NKGASGDSYT
421 LSLSGAGYTA GQQLTEVIGC TTVTVGSDGN
451 VPVPMAGGLP RVLYPTEKLA GSKICSSS

1	CB	VAL A	1	11.902	27.157	22.095	1.00	23.86	6	54	CB	TYR A	8	28.238	37.382	24.476	1.00	10.19	6
2	CG1	VAL A	1	12.302	27.494	20.658	1.00	24.08	6	55	CG	TYR A	8	27.909	38.377	23.351	1.00	10.76	6
3	CG2	VAL A	1	10.659	27.948	22.511	1.00	26.37	6	56	CD1	TYR A	8	27.180	37.983	22.222	1.00	11.00	6
4	C	VAL A	1	13.030	25.096	22.743	1.00	19.54	6	57	CE1	TYR A	8	26.891	38.842	21.190	1.00	11.22	6
5	O	VAL A	1	13.191	25.013	23.967	1.00	19.86	8	58	CD2	TYR A	8	28.340	39.698	23.424	1.00	10.96	6
6	H	VAL A	1	10.702	25.241	23.415	1.00	20.28	7	59	CE2	TYR A	8	28.080	40.620	22.423	1.00	11.25	6
7	CA	VAL A	1	11.659	25.658	22.335	1.00	20.25	6	60	C2	TYR A	8	27.358	40.156	21.312	1.00	11.62	6
8	H	ASH A	2	13.867	24.729	21.802	1.00	18.39	7	61	OH	TYR A	8	27.114	41.063	20.294	1.00	11.87	8
9	CA	ASH A	2	15.168	24.197	22.212	1.00	16.73	6	62	C	TYR A	8	30.789	37.289	24.119	1.00	9.70	6
10	CB	ASH A	2	15.836	23.657	20.945	1.00	16.09	6	63	O	TYR A	8	30.918	38.427	24.563	1.00	9.67	8
11	CG	ASH A	2	15.219	22.336	20.451	1.00	15.33	6	64	H	PIE A	9	31.890	36.710	23.639	1.00	9.16	7
12	CD1	ASH A	2	14.707	21.549	21.252	1.00	15.28	8	65	CA	PIE A	9	33.191	37.307	23.588	1.00	9.15	6
13	HD2	ASH A	2	15.283	22.082	19.151	1.00	12.41	7	66	CB	PIE A	9	33.805	37.750	24.941	1.00	8.08	6
14	C	ASH A	2	15.969	25.334	22.767	1.00	15.71	6	67	CG	PIE A	9	33.968	36.659	25.978	1.00	9.21	6
15	O	ASH A	2	15.903	26.435	22.198	1.00	16.02	8	68	CD1	PIE A	9	35.239	36.125	26.240	1.00	10.15	6
16	H	GLY A	3	16.720	25.198	23.833	1.00	14.56	7	69	CD2	PIE A	9	32.887	36.171	26.720	1.00	7.79	6
17	CA	GLY A	3	17.541	26.305	24.331	1.00	13.21	6	70	CE1	PIE A	9	35.440	35.161	27.245	1.00	10.23	6
18	C	GLY A	3	18.940	26.211	23.671	1.00	12.14	6	71	CE2	PIE A	9	33.070	35.205	27.669	1.00	7.64	6
19	O	GLY A	3	19.498	25.153	23.302	1.00	11.92	8	72	C2	PIE A	9	34.313	34.698	27.962	1.00	8.17	6
20	H	THR A	4	20.829	27.555	22.912	1.00	10.96	6	73	C	PIE A	9	34.173	36.294	22.963	1.00	8.94	6
21	CA	THR A	4	19.503	27.368	23.499	1.00	11.28	7	74	O	PIE A	9	33.903	35.102	22.918	1.00	8.65	8
22	CB	THR A	4	20.721	27.878	21.400	1.00	11.09	6	75	H	GLU A	10	35.284	36.856	22.536	1.00	9.09	7
23	CG1	THR A	4	19.920	26.828	20.782	1.00	12.31	8	76	CA	GLU A	10	36.430	36.089	22.006	1.00	9.38	6
24	CG2	THR A	4	22.048	27.933	20.693	1.00	8.99	6	77	CB	GLU A	10	36.508	36.043	20.513	1.00	7.45	6
25	C	THR A	4	21.584	28.664	23.663	1.00	10.56	6	78	CG	GLU A	10	36.604	37.345	19.740	1.00	7.55	6
26	O	THR A	4	21.080	29.743	23.866	1.00	9.98	8	79	CD	GLU A	10	37.981	37.580	19.156	1.00	6.81	6
27	H	LEU A	5	22.809	28.376	24.092	1.00	10.63	7	80	OE1	GLU A	10	38.145	38.544	18.397	1.00	8.43	8
28	CA	LEU A	5	23.700	29.291	24.818	1.00	10.69	6	81	OE2	GLU A	10	38.962	36.877	19.438	1.00	5.00	8
29	CB	LEU A	5	24.515	28.477	25.789	1.00	9.31	6	82	C	GLU A	10	37.636	36.715	22.737	1.00	9.90	6
30	CG	LEU A	5	25.429	28.946	26.864	1.00	10.96	6	83	O	GLU A	10	37.590	37.807	23.361	1.00	9.92	8
31	CD1	LEU A	5	24.887	30.150	27.608	1.00	9.46	6	84	H	TRP A	11	38.791	36.059	22.729	1.00	10.15	7
32	CD2	LEU A	5	25.608	27.802	27.884	1.00	10.55	6	85	CA	TRP A	11	39.980	36.551	23.407	1.00	10.35	6
33	C	LEU A	5	24.644	29.992	23.840	1.00	10.85	6	86	CB	TRP A	11	41.182	35.619	23.186	1.00	9.98	6
34	O	LEU A	5	25.047	29.453	22.799	1.00	10.85	8	87	CG	TRP A	11	42.271	35.940	24.181	1.00	11.61	6
35	H	HET A	6	25.031	31.217	24.123	1.00	10.88	7	88	CD2	TRP A	11	42.292	35.583	25.565	1.00	12.44	6
36	CA	HET A	6	25.971	31.930	23.312	1.00	12.97	6	89	CE2	TRP A	11	43.516	36.063	26.103	1.00	12.84	6
37	CB	HET A	6	25.455	33.143	22.507	1.00	10.94	6	90	CE3	TRP A	11	41.412	34.916	26.432	1.00	13.39	6
38	CG	HET A	6	26.629	33.643	21.638	1.00	15.17	6	91	CD1	TRP A	11	43.446	36.606	23.915	1.00	11.78	6
39	SD	HET A	6	26.027	34.480	20.185	1.00	19.39	16	92	HE1	TRP A	11	44.188	36.673	25.083	1.00	12.99	7
40	CE	HET A	6	27.525	35.144	19.516	1.00	16.94	6	93	C22	TRP A	11	43.831	35.890	27.441	1.00	13.37	6
41	C	HET A	6	27.089	32.485	24.223	1.00	10.67	6	94	C23	TRP A	11	41.717	34.763	27.772	1.00	13.91	6
42	O	HET A	6	26.774	33.206	25.170	1.00	10.51	8	95	CN2	TRP A	11	42.946	35.256	28.280	1.00	14.23	6
43	H	GLN A	7	28.325	32.133	23.911	1.00	10.34	7	96	C	TRP A	11	40.410	37.937	22.933	1.00	10.57	6
44	CA	GLN A	7	29.440	32.727	24.681	1.00	10.20	6	97	O	TRP A	11	40.843	38.709	23.797	1.00	10.47	8
45	CB	GLN A	7	30.696	31.910	24.617	1.00	9.41	6	98	H	TYR A	12	40.322	38.209	21.623	1.00	10.73	7
46	CD	GLN A	7	31.967	32.632	25.053	1.00	10.26	6	99	CA	TYR A	12	40.766	39.508	21.126	1.00	11.11	6
47	OE1	GLN A	7	33.280	31.914	25.027	1.00	9.15	6	100	CB	TYR A	12	41.559	39.432	19.798	1.00	11.11	6
48	HE2	GLN A	7	34.327	32.470	25.449	1.00	12.35	8	101	CG	TYR A	12	42.765	38.515	20.029	1.00	11.60	6
49	GLN A	7	33.359	30.714	24.570	1.00	6.58	7	102	CD1	TYR A	12	42.605	37.158	19.704	1.00	11.95	6	
50	O	GLN A	7	29.578	34.125	24.015	1.00	10.22	6	103	CE1	TYR A	12	43.666	36.268	19.892	1.00	12.43	6
51	C	GLN A	7	29.856	34.167	22.786	1.00	10.30	8	104	CD2	TYR A	12	43.985	38.951	20.540	1.00	11.48	6
52	H	TYR A	8	29.394	35.236	24.691	1.00	9.97	7	105	CE2	TYR A	12	45.023	38.076	20.714	1.00	11.85	6
53	CA	TYR A	8	29.467	36.526	24.022	1.00	9.95	6	106	CZ	TYR A	12	44.870	36.749	20.388	1.00	12.61	6

107	ATOH	OH	TYR A	12	45.854	35.787	20.560	1.00	13.18	8	160	NE2	HIS A	19	31.584	41.112	24.073	1.00	9.42	7
108	ATOH	C	TYR A	12	39.687	40.574	20.991	1.00	11.38	6	161	C	HIS A	19	30.007	45.489	25.132	1.00	9.04	6
109	ATOH	O	TYR A	12	39.862	41.436	20.132	1.00	11.53	8	162	O	HIS A	19	29.153	44.838	24.493	1.00	8.75	8
110	ATOH	H	THR A	13	38.630	40.547	21.783	1.00	11.49	7	163	H	TRP A	20	29.650	46.184	26.217	1.00	9.17	7
111	ATOH	CA	THR A	13	37.651	41.656	21.700	1.00	11.50	6	164	CA	TRP A	20	28.248	46.090	26.688	1.00	9.56	6
112	ATOH	CA	THR A	13	36.604	41.321	22.761	1.00	13.32	6	165	CA	TRP A	20	28.200	46.691	28.093	1.00	8.24	6
113	ATOH	OG1	THR A	13	35.755	40.296	22.169	1.00	14.85	8	166	CG	TRP A	20	29.112	46.119	29.122	1.00	7.50	6
114	ATOH	CG2	THR A	13	35.732	42.466	23.175	1.00	14.00	6	167	CG2	TRP A	20	29.515	44.774	29.341	1.00	7.46	6
115	ATOH	C	THR A	13	38.489	42.880	22.036	1.00	11.41	6	168	CE2	TRP A	20	30.374	44.751	30.459	1.00	7.35	6
116	ATOH	O	THR A	13	39.429	42.805	22.840	1.00	11.13	8	169	CE3	TRP A	20	29.187	43.568	28.695	1.00	8.23	6
117	ATOH	H	PRO A	14	38.254	44.015	21.408	1.00	11.47	7	170	CO1	TRP A	20	29.736	46.854	30.088	1.00	7.37	6
118	ATOH	CO	PRO A	14	37.184	44.144	20.397	1.00	11.68	6	171	NE1	TRP A	20	30.483	46.041	30.920	1.00	7.58	7
119	ATOH	CA	PRO A	14	38.979	45.243	21.611	1.00	11.44	6	172	C22	TRP A	20	30.926	43.591	31.006	1.00	6.78	6
120	ATOH	CB	PRO A	14	38.477	46.296	20.569	1.00	11.60	6	173	C23	TRP A	20	29.750	42.407	29.223	1.00	7.26	6
121	ATOH	CG	PRO A	14	37.352	45.564	19.896	1.00	11.77	6	174	CH2	TRP A	20	30.608	42.427	30.366	1.00	7.69	6
122	ATOH	C	PRO A	14	38.786	45.868	22.993	1.00	11.21	6	175	C	TRP A	20	27.227	46.746	25.757	1.00	9.73	6
123	ATOH	O	PRO A	14	37.703	45.785	23.618	1.00	11.15	8	176	O	TRP A	20	26.070	46.395	25.592	1.00	9.42	8
124	ATOH	H	ASN A	15	39.806	46.557	23.445	1.00	10.84	7	177	H	LYS A	21	27.591	47.832	25.102	1.00	10.37	7
125	ATOH	CA	ASN A	15	39.720	47.304	24.693	1.00	11.02	6	178	CA	LYS A	21	26.731	48.544	24.144	1.00	11.41	6
126	ATOH	CB	ASN A	15	41.073	47.318	25.411	1.00	11.27	6	179	CB	LYS A	21	27.348	49.856	23.671	1.00	15.11	6
127	ATOH	CG	ASN A	15	41.055	48.247	26.614	1.00	11.89	6	180	CG	LYS A	21	27.086	50.981	24.674	1.00	21.25	6
128	ATOH	OO1	ASN A	15	40.008	48.358	27.277	1.00	12.57	8	181	CG	LYS A	21	28.020	52.128	24.411	1.00	25.92	6
129	ATOH	H02	ASN A	15	42.158	48.898	26.922	1.00	11.38	7	182	CE	LYS A	21	27.600	53.426	25.067	1.00	30.86	6
130	ATOH	C	ASN A	15	39.240	48.737	24.377	1.00	11.05	6	183	NZ	LYS A	21	27.119	54.448	24.030	1.00	34.41	7
131	ATOH	O	ASN A	15	39.932	49.767	24.524	1.00	11.08	8	184	C	LYS A	21	26.551	47.632	22.934	1.00	11.59	6
132	ATOH	N	ASP A	16	38.008	48.835	23.905	1.00	10.98	7	185	O	LYS A	21	25.474	47.562	22.400	1.00	11.87	7
133	ATOH	CA	ASP A	16	37.446	50.118	23.529	1.00	11.17	6	186	N	ARG A	22	27.626	46.953	22.545	1.00	12.42	6
134	ATOH	CB	ASP A	16	36.924	50.059	22.068	1.00	11.99	6	187	CB	ARG A	22	27.576	46.015	21.451	1.00	12.84	6
135	ATOH	CG	ASP A	16	35.761	49.101	21.873	1.00	12.89	6	188	CA	ARG A	22	28.940	45.391	21.199	1.00	13.26	6
136	ATOH	OO1	ASP A	16	35.313	48.341	22.772	1.00	11.83	8	189	CG	ARG A	22	29.804	46.215	20.240	1.00	14.04	7
137	ATOH	O02	ASP A	16	35.244	49.114	20.732	1.00	14.31	8	190	CO	ARG A	22	31.043	45.363	19.942	1.00	14.67	6
138	ATOH	C	ASP A	16	36.352	50.518	24.498	1.00	11.03	6	191	NE	ARG A	22	32.084	45.253	20.955	1.00	14.04	7
139	ATOH	O	ASP A	16	35.768	51.582	24.289	1.00	11.12	8	192	CZ	ARG A	22	33.068	46.161	21.065	1.00	14.66	6
140	ATOH	H	GLY A	17	36.013	49.732	25.513	1.00	10.89	7	193	NH1	ARG A	22	33.913	45.855	22.063	1.00	13.42	7
141	ATOH	CA	GLY A	17	34.972	50.083	26.479	1.00	10.61	6	194	NH2	ARG A	22	33.206	47.242	20.261	1.00	12.34	7
142	ATOH	C	GLY A	17	33.545	50.032	25.938	1.00	10.65	6	195	O	ARG A	22	26.586	44.921	21.812	1.00	12.77	6
143	ATOH	O	GLY A	17	32.629	50.522	26.601	1.00	10.67	8	196	O	ARG A	22	25.682	44.543	21.038	1.00	13.11	8
144	ATOH	N	GLN A	18	33.287	49.436	24.766	1.00	10.50	7	197	N	LEU A	23	26.678	44.342	23.002	1.00	12.84	7
145	ATOH	CA	GLN A	18	31.995	49.346	24.151	1.00	10.55	6	198	CA	LEU A	23	25.698	43.292	23.370	1.00	12.86	6
146	ATOH	CB	GLN A	18	32.064	49.835	22.691	1.00	15.25	6	199	CB	LEU A	23	26.092	42.716	24.721	1.00	10.68	6
147	ATOH	CG	GLN A	18	32.718	51.182	22.436	1.00	21.24	6	200	CG	LEU A	23	25.126	41.739	25.361	1.00	10.16	6
148	ATOH	CO	GLN A	18	31.729	52.313	22.693	1.00	25.84	6	201	CO1	LEU A	23	24.804	40.562	24.449	1.00	8.43	6
149	ATOH	OE1	GLN A	18	30.674	52.415	22.016	1.00	29.22	8	202	CO2	LEU A	23	25.769	41.258	26.669	1.00	9.16	6
150	ATOH	HE2	GLN A	18	32.104	53.124	23.668	1.00	27.29	7	203	C	LEU A	23	24.285	43.874	22.388	1.00	13.25	6
151	ATOH	C	GLN A	18	31.421	47.936	24.042	1.00	10.04	6	204	O	LEU A	23	23.302	43.247	22.969	1.00	12.84	8
152	ATOH	O	GLN A	18	30.467	47.808	23.281	1.00	9.96	8	205	N	GLN A	24	24.144	45.123	23.873	1.00	13.66	7
153	ATOH	H	HIS A	19	31.986	46.944	24.702	1.00	9.66	7	206	CA	GLN A	24	22.848	45.781	23.929	1.00	14.44	6
154	ATOH	CA	HIS A	19	31.440	45.572	24.582	1.00	9.29	6	207	CB	GLN A	24	22.959	47.205	24.523	1.00	16.30	6
155	ATOH	CB	HIS A	19	32.412	44.535	25.162	1.00	6.70	6	208	CG	GLN A	24	21.578	47.851	24.620	1.00	18.17	6
156	ATOH	CG	HIS A	19	32.091	43.173	24.563	1.00	8.79	6	209	CO	GLN A	24	21.659	49.208	25.296	1.00	20.30	6
157	ATOH	CO2	HIS A	19	31.749	41.987	25.138	1.00	7.93	6	210	OE1	GLN A	24	22.651	49.936	25.205	1.00	21.20	8
158	ATOH	H01	HIS A	19	32.116	42.955	23.187	1.00	8.36	7	211	HE2	GLN A	24	20.619	49.539	26.023	1.00	20.53	7
159	ATOH	CE1	HIS A	19	31.825	41.705	22.909	1.00	8.32	6	212	C	GLN A	24	22.208	45.914	22.528	1.00	14.70	6

213	ATOH	O	GLU A	24	21.030	45.626	22.296	1.00	14.63	8
214	ATOH	H	ASH A	25	23.034	46.369	21.594	1.00	14.90	7
215	ATOH	CA	ASH A	25	22.642	46.525	20.213	1.00	15.31	6
216	ATOH	CB	ASH A	25	23.645	47.256	19.304	1.00	18.01	6
217	ATOH	CG	ASH A	25	23.711	48.719	19.680	1.00	22.28	6
218	ATOH	001	ASH A	25	22.686	49.238	20.127	1.00	24.44	6
219	ATOH	H02	ASH A	25	24.836	49.432	19.588	1.00	23.11	7
220	ATOH	C	ASH A	25	22.371	45.141	19.588	1.00	15.19	6
221	ATOH	O	ASH A	25	21.542	45.198	18.637	1.00	15.31	8
222	ATOH	H	ASP A	26	22.954	44.059	20.051	1.00	14.67	7
223	ATOH	CA	ASP A	26	22.647	42.765	19.394	1.00	14.48	6
224	ATOH	CB	ASP A	26	24.002	42.002	19.440	1.00	14.63	6
225	ATOH	CG	ASP A	26	24.340	41.059	18.322	1.00	14.74	6
226	ATOH	001	ASP A	26	23.651	41.073	17.292	1.00	14.77	8
227	ATOH	H02	ASP A	26	25.294	40.238	18.363	1.00	14.65	8
228	ATOH	C	ASP A	26	21.497	41.933	19.949	1.00	14.18	6
229	ATOH	O	ASP A	26	21.119	40.869	19.454	1.00	13.76	8
230	ATOH	H	ALA A	27	20.813	42.356	20.986	1.00	14.32	7
231	ATOH	CA	ALA A	27	19.761	41.641	21.661	1.00	14.78	6
232	ATOH	CB	ALA A	27	19.276	42.463	22.849	1.00	12.97	6
233	ATOH	C	ALA A	27	18.627	41.207	20.754	1.00	15.34	6
234	ATOH	O	ALA A	27	18.231	40.028	20.840	1.00	15.56	8
235	ATOH	H	GLU A	28	18.099	42.032	19.858	1.00	15.76	7
236	ATOH	CA	GLU A	28	17.010	41.598	18.984	1.00	16.05	6
237	ATOH	CB	GLU A	28	16.526	42.815	18.170	1.00	23.00	6
238	ATOH	CG	GLU A	28	15.097	42.736	17.596	1.00	31.01	6
239	ATOH	001	GLU A	28	14.001	42.258	18.567	1.00	36.48	6
240	ATOH	OE1	GLU A	28	13.644	41.013	18.587	1.00	40.16	8
241	ATOH	OE2	GLU A	28	13.427	43.089	19.316	1.00	38.33	8
242	ATOH	C	GLU A	28	17.410	40.467	18.044	1.00	15.55	6
243	ATOH	O	GLU A	28	16.773	39.435	17.835	1.00	15.27	8
244	ATOH	H	HIS A	29	18.577	40.712	17.415	1.00	15.36	7
245	ATOH	CA	HIS A	29	19.158	39.769	16.461	1.00	15.11	6
246	ATOH	CB	HIS A	29	20.492	40.422	16.008	1.00	16.22	6
247	ATOH	CG	HIS A	29	21.296	39.400	15.259	1.00	18.29	6
248	ATOH	001	HIS A	29	20.895	38.501	14.294	1.00	18.16	6
249	ATOH	H01	HIS A	29	22.639	39.155	15.496	1.00	18.52	7
250	ATOH	CE1	HIS A	29	23.055	38.163	14.693	1.00	18.61	6
251	ATOH	HE2	HIS A	29	22.006	37.741	13.984	1.00	18.61	7
252	ATOH	C	HIS A	29	19.282	38.370	17.059	1.00	14.84	6
253	ATOH	O	HIS A	29	18.852	37.340	16.543	1.00	14.68	8
254	ATOH	H	LEU A	30	19.913	38.292	18.233	1.00	14.66	7
255	ATOH	CA	LEU A	30	20.154	37.107	19.020	1.00	14.56	6
256	ATOH	CB	LEU A	30	20.913	37.409	20.319	1.00	13.60	6
257	ATOH	CG	LEU A	30	22.350	37.884	20.194	1.00	15.90	6
258	ATOH	001	LEU A	30	23.018	37.967	21.586	1.00	15.00	6
259	ATOH	002	LEU A	30	18.833	36.434	19.292	1.00	14.94	6
260	ATOH	C	LEU A	30	18.033	35.228	19.390	1.00	14.68	6
261	ATOH	O	LEU A	30	17.877	37.240	19.879	1.00	15.37	7
262	ATOH	H	SER A	31	16.596	36.559	20.204	1.00	16.15	6
263	ATOH	CA	SER A	31	15.603	37.378	21.005	1.00	17.82	6
264	ATOH	CB	SER A	31	15.358	38.528	20.190	1.00	22.98	8
265	ATOH	OG	SER A	31						
266	ATOH	C	SER A	31						
267	ATOH	O	SER A	31						
268	ATOH	H	ASP A	32						
269	ATOH	CA	ASP A	32						
270	ATOH	CB	ASP A	32						
271	ATOH	CG	ASP A	32						
272	ATOH	001	ASP A	32						
273	ATOH	002	ASP A	32						
274	ATOH	C	ASP A	32						
275	ATOH	O	ASP A	32						
276	ATOH	N	ILE A	33						
277	ATOH	CA	ILE A	33						
278	ATOH	CB	ILE A	33						
279	ATOH	CG2	ILE A	33						
280	ATOH	CG1	ILE A	33						
281	ATOH	CD1	ILE A	33						
282	ATOH	C	ILE A	33						
283	ATOH	O	ILE A	33						
284	ATOH	N	GLY A	34						
285	ATOH	CA	GLY A	34						
286	ATOH	C	GLY A	34						
287	ATOH	O	GLY A	34						
288	ATOH	N	ILE A	35						
289	ATOH	CA	ILE A	35						
290	ATOH	CB	ILE A	35						
291	ATOH	CG2	ILE A	35						
292	ATOH	CG1	ILE A	35						
293	ATOH	CD1	ILE A	35						
294	ATOH	C	ILE A	35						
295	ATOH	O	ILE A	35						
296	ATOH	N	THR A	36						
297	ATOH	CA	THR A	36						
298	ATOH	CB	THR A	36						
299	ATOH	OG1	THR A	36						
300	ATOH	CG2	THR A	36						
301	ATOH	C	THR A	36						
302	ATOH	O	THR A	36						
303	ATOH	N	ALA A	37						
304	ATOH	CA	ALA A	37						
305	ATOH	CB	ALA A	37						
306	ATOH	C	ALA A	37						
307	ATOH	O	ALA A	37						
308	ATOH	N	VAL A	38						
309	ATOH	CA	VAL A	38						
310	ATOH	CB	VAL A	38						
311	ATOH	CG2	VAL A	38						
312	ATOH	CG1	VAL A	38						
313	ATOH	C	VAL A	38						
314	ATOH	O	VAL A	38						
315	ATOH	N	TRP A	39						
316	ATOH	CA	TRP A	39						
317	ATOH	CB	TRP A	39						
318	ATOH	CG	TRP A	39						

ATOM	319	CD2	TRP	A	39	30.691	31.682	28.807	1.00	6.00	6	ATOM	372	CD	LYS	A	45	39.093	48.021	37.024	1.00	5.00	6
ATOM	320	CE2	TRP	A	39	31.875	32.074	29.473	1.00	5.58	6	ATOM	373	CE	LYS	A	45	37.830	48.865	36.976	1.00	5.00	6
ATOM	321	CE3	TRP	A	39	30.708	30.585	27.908	1.00	5.00	6	ATOM	374	N2	LYS	A	45	37.599	49.990	37.908	1.00	5.00	7
ATOM	322	CD1	TRP	A	39	30.201	33.372	30.190	1.00	5.74	6	ATOM	375	C	LYS	A	45	39.029	44.010	37.657	1.00	5.87	6
ATOM	323	HE1	TRP	A	39	31.568	33.153	30.268	1.00	5.57	7	ATOM	376	N	LYS	A	45	39.207	43.306	38.636	1.00	5.70	8
ATOM	324	C22	TRP	A	39	33.099	31.441	29.211	1.00	5.00	6	ATOM	377	H	GLY	A	46	39.847	43.978	36.608	1.00	6.09	7
ATOM	325	C23	TRP	A	39	31.955	29.964	27.701	1.00	5.00	6	ATOM	378	CA	GLY	A	46	41.017	43.149	36.478	1.00	6.70	6
ATOM	326	CH2	TRP	A	39	33.115	30.400	28.307	1.00	5.00	6	ATOM	379	C	GLY	A	46	42.246	43.917	36.957	1.00	7.41	6
ATOM	327	C	TRP	A	39	28.317	35.078	28.452	1.00	8.53	6	ATOM	380	O	GLY	A	46	42.171	45.098	37.382	1.00	7.54	8
ATOM	328	O	TRP	A	39	28.856	35.399	27.384	1.00	8.32	8	ATOM	381	H	LEU	A	47	43.420	43.291	36.970	1.00	7.77	7
ATOM	329	H	ILE	A	40	28.431	35.945	29.459	1.00	8.37	7	ATOM	382	CA	LEU	A	47	44.681	43.889	37.385	1.00	8.34	6
ATOM	330	CA	ILE	A	40	29.143	37.247	29.667	1.00	8.51	6	ATOM	383	CB	LEU	A	47	45.838	42.922	37.455	1.00	9.18	6
ATOM	331	CB	ILE	A	40	28.091	38.113	30.259	1.00	9.85	6	ATOM	384	CG	LEU	A	47	46.426	42.140	36.297	1.00	11.32	6
ATOM	332	CG2	ILE	A	40	28.089	38.802	31.613	1.00	9.64	6	ATOM	385	CG	LEU	A	47	45.419	41.207	35.660	1.00	12.40	6
ATOM	333	CG1	ILE	A	40	27.803	39.287	29.286	1.00	9.52	6	ATOM	386	CD2	LEU	A	47	46.897	42.995	35.137	1.00	12.34	6
ATOM	334	CD1	ILE	A	40	26.594	38.637	28.616	1.00	11.76	6	ATOM	387	C	LEU	A	47	45.040	45.105	36.483	1.00	8.70	6
ATOM	335	C	ILE	A	40	30.524	37.121	30.063	1.00	8.39	6	ATOM	388	O	LEU	A	47	45.884	45.929	36.872	1.00	8.67	8
ATOM	336	O	ILE	A	40	30.680	36.373	31.033	1.00	8.04	8	ATOM	389	N	SER	A	48	44.451	45.283	35.303	1.00	8.86	7
ATOM	337	H	PRO	A	41	31.571	37.800	29.564	1.00	8.30	7	ATOM	390	CA	SER	A	48	44.667	46.453	34.457	1.00	9.11	6
ATOM	338	CD	PRO	A	41	31.469	38.773	28.451	1.00	8.06	6	ATOM	391	CG	SER	A	48	45.870	46.312	33.492	1.00	9.17	6
ATOM	339	CA	PRO	A	41	32.887	37.771	30.151	1.00	8.14	6	ATOM	392	OG	SER	A	48	45.546	45.387	32.490	1.00	8.88	8
ATOM	340	CB	PRO	A	41	33.802	38.683	29.246	1.00	8.13	6	ATOM	393	C	SER	A	48	43.380	46.678	33.672	1.00	9.13	6
ATOM	341	CG	PRO	A	41	32.756	39.565	28.595	1.00	8.01	6	ATOM	394	O	SER	A	48	42.533	45.777	33.610	1.00	9.05	8
ATOM	342	C	PRO	A	41	32.846	38.312	31.590	1.00	7.87	6	ATOM	395	N	GLN	A	49	43.225	47.807	33.003	1.00	9.23	7
ATOM	343	O	PRO	A	41	31.891	38.952	32.039	1.00	7.72	8	ATOM	396	CA	GLN	A	49	42.076	48.113	32.174	1.00	9.17	6
ATOM	344	H	PRO	A	42	33.909	38.044	32.341	1.00	7.64	7	ATOM	397	CB	GLN	A	49	42.104	49.549	31.592	1.00	6.81	6
ATOM	345	CD	PRO	A	42	35.113	37.297	31.880	1.00	7.36	6	ATOM	398	CG	GLN	A	49	40.813	49.921	30.864	1.00	5.86	6
ATOM	346	CA	PRO	A	42	34.084	38.542	33.711	1.00	7.41	6	ATOM	399	CD	GLN	A	49	41.078	51.178	30.041	1.00	7.48	6
ATOM	347	CB	PRO	A	42	35.490	38.085	34.191	1.00	7.45	6	ATOM	400	OE1	GLN	A	49	41.898	51.153	29.103	1.00	7.62	8
ATOM	348	CG	PRO	A	42	35.772	36.947	33.217	1.00	7.45	6	ATOM	401	NE2	GLN	A	49	40.489	52.278	30.467	1.00	5.00	7
ATOM	349	C	PRO	A	42	33.841	40.054	33.685	1.00	7.06	6	ATOM	402	C	GLN	A	49	41.929	47.121	31.006	1.00	9.30	6
ATOM	350	O	PRO	A	42	34.481	40.819	32.931	1.00	6.95	8	ATOM	403	O	GLN	A	49	40.774	46.745	30.647	1.00	9.52	8
ATOM	351	H	ALA	A	43	32.875	40.536	34.452	1.00	6.53	7	ATOM	404	N	SER	A	50	43.038	46.690	30.424	1.00	9.20	7
ATOM	352	CA	ALA	A	43	32.477	41.937	34.481	1.00	6.39	6	ATOM	405	CA	SER	A	50	42.992	45.763	29.281	1.00	9.33	6
ATOM	353	CB	ALA	A	43	30.968	41.991	34.756	1.00	5.00	6	ATOM	406	CB	SER	A	50	44.173	46.116	28.346	1.00	11.13	6
ATOM	354	C	ALA	A	43	33.131	42.845	35.529	1.00	6.36	6	ATOM	407	OG	SER	A	50	45.417	45.891	29.000	1.00	14.96	8
ATOM	355	O	ALA	A	43	32.847	44.042	35.582	1.00	6.42	8	ATOM	408	C	SER	A	50	42.924	44.272	29.626	1.00	8.88	6
ATOM	356	N	TYR	A	44	33.995	42.333	36.394	1.00	6.22	7	ATOM	409	O	SER	A	50	42.810	43.409	28.736	1.00	8.96	8
ATOM	357	CA	TYR	A	44	34.637	43.052	37.465	1.00	6.10	6	ATOM	410	H	ASP	A	51	42.910	43.891	30.881	1.00	8.41	7
ATOM	358	CB	TYR	A	44	34.455	42.266	38.819	1.00	6.31	6	ATOM	411	CB	ASP	A	51	42.812	42.467	31.211	1.00	7.98	6
ATOM	359	CG	TYR	A	44	34.381	40.781	38.551	1.00	6.51	6	ATOM	412	CA	ASP	A	51	43.030	42.303	32.724	1.00	7.44	6
ATOM	360	CD1	TYR	A	44	35.538	40.086	38.145	1.00	6.67	6	ATOM	413	CG	ASP	A	51	43.044	40.822	33.120	1.00	8.58	6
ATOM	361	CE1	TYR	A	44	35.472	38.732	37.848	1.00	6.66	6	ATOM	414	CD1	ASP	A	51	44.069	40.115	32.869	1.00	8.63	8
ATOM	362	CE2	TYR	A	44	33.200	40.071	38.613	1.00	6.52	6	ATOM	415	CD2	ASP	A	51	41.992	40.399	33.679	1.00	8.06	8
ATOM	363	CE2	TYR	A	44	33.108	38.722	38.301	1.00	6.55	6	ATOM	416	C	ASP	A	51	41.460	41.932	30.766	1.00	7.80	6
ATOM	364	C	TYR	A	44	34.276	38.073	37.917	1.00	6.98	6	ATOM	417	O	ASP	A	51	40.441	42.613	30.990	1.00	7.70	8
ATOM	365	OH	TYR	A	44	34.209	36.729	37.568	1.00	7.43	8	ATOM	418	H	ASN	A	52	41.330	40.729	30.217	1.00	7.56	7
ATOM	366	C	TYR	A	44	36.060	43.413	37.075	1.00	5.99	6	ATOM	419	CA	ASN	A	52	40.040	40.182	29.867	1.00	9.45	6
ATOM	367	O	TYR	A	44	36.682	42.945	36.097	1.00	5.98	8	ATOM	420	CB	ASN	A	52	40.175	38.887	29.057	1.00	12.85	6
ATOM	368	H	LYS	A	45	36.556	44.410	37.815	1.00	5.93	7	ATOM	421	CG	ASN	A	52	40.562	39.187	27.620	1.00	15.76	8
ATOM	369	CA	LYS	A	45	37.865	45.003	37.567	1.00	5.73	6	ATOM	422	CG	ASN	A	52	40.516	40.341	27.167	1.00	12.70	7
ATOM	370	CB	LYS	A	45	38.033	46.160	38.580	1.00	5.00	6	ATOM	423	HD2	ASN	A	52	40.979	38.239	26.786	1.00	7.16	6
ATOM	371	CG	LYS	A	45	39.192	47.127	38.251	1.00	5.00	6	ATOM	424	C	ASN	A	52	39.166	39.829	31.071	1.00	7.16	6

ATOM	425	O	ASN A	52	38.007	39.399	30.782	1.00	7.11	8	ATOM	478	CD2 LEU A	59	35.960	38.571	41.423	1.00	6.96	6	
ATOM	426	N	GLY A	53	39.652	39.949	32.309	1.00	6.67	7	ATOM	479	C	LEU A	59	33.758	42.311	42.650	1.00	5.05	6
ATOM	427	CA	GLY A	53	38.832	39.609	33.457	1.00	6.52	6	ATOM	480	O	LEU A	59	32.644	42.112	42.100	1.00	5.00	8
ATOM	428	C	GLY A	53	39.262	38.324	34.124	1.00	6.62	6	ATOM	481	N	TYR A	60	33.921	43.352	43.480	1.00	5.25	7
ATOM	429	O	GLY A	53	38.726	38.021	35.199	1.00	6.84	8	ATOM	482	CA	TYR A	60	32.804	44.266	43.786	1.00	5.52	6
ATOM	430	N	TYR A	54	40.227	37.565	33.548	1.00	6.28	7	ATOM	483	CB	TYR A	60	32.811	44.611	45.271	1.00	5.24	6
ATOM	431	CA	TYR A	54	40.722	36.331	34.179	1.00	5.98	6	ATOM	484	CG	TYR A	60	32.214	43.597	46.224	1.00	5.38	6
ATOM	432	CB	TYR A	54	41.027	35.227	33.116	1.00	6.06	6	ATOM	485	CD1 TYR A	60	33.101	42.761	46.929	1.00	5.65	6	
ATOM	433	CG	TYR A	54	39.720	34.834	32.427	1.00	5.99	6	ATOM	486	CE1 TYR A	60	32.646	41.833	47.866	1.00	5.89	6	
ATOM	434	CD1 TYR A	54	39.481	35.232	31.108	1.00	6.44	6	ATOM	487	CD2 TYR A	60	30.855	43.441	46.441	1.00	5.22	6		
ATOM	435	CE1 TYR A	54	38.251	34.920	30.492	1.00	6.68	6	ATOM	488	CE2 TYR A	60	30.359	42.520	47.333	1.00	5.60	6		
ATOM	436	CD2 TYR A	54	38.700	34.194	33.088	1.00	5.97	6	ATOM	489	C2 TYR A	60	31.255	41.742	48.063	1.00	6.27	6		
ATOM	437	CE2 TYR A	54	37.474	33.857	32.517	1.00	6.05	6	ATOM	490	OH	TYR A	60	30.867	40.764	48.957	1.00	6.71	8	
ATOM	438	C2 TYR A	54	37.282	34.209	31.182	1.00	6.50	6	ATOM	491	C	TYR A	60	32.888	45.540	42.937	1.00	5.77	6	
ATOM	439	OH	TYR A	54	36.083	33.928	30.558	1.00	6.69	8	ATOM	492	O	TYR A	60	32.117	46.467	43.158	1.00	6.16	8
ATOM	440	C	TYR A	54	41.879	36.549	35.145	1.00	5.76	6	ATOM	493	N	ASP A	61	33.824	45.690	42.052	1.00	5.53	7
ATOM	441	O	TYR A	54	42.441	35.655	35.818	1.00	5.63	8	ATOM	494	CA	ASP A	61	33.963	46.831	41.196	1.00	5.82	6
ATOM	442	N	GLY A	55	42.237	37.799	35.429	1.00	5.53	7	ATOM	495	CB	ASP A	61	35.395	47.325	41.096	1.00	5.00	6
ATOM	443	CA	GLY A	55	43.226	38.205	36.438	1.00	5.64	6	ATOM	496	CG	ASP A	61	35.635	48.569	40.256	1.00	5.28	6
ATOM	444	C	GLY A	55	42.464	39.315	37.256	1.00	5.59	6	ATOM	497	OO1 ASP A	61	34.717	49.013	39.468	1.00	6.54	8	
ATOM	445	O	GLY A	55	42.818	40.499	37.213	1.00	5.60	8	ATOM	498	OO2 ASP A	61	36.778	49.132	40.283	1.00	5.00	8	
ATOM	446	N	PRO A	56	41.410	38.876	37.948	1.00	5.20	7	ATOM	499	C	ASP A	61	33.455	46.390	39.790	1.00	6.20	6
ATOM	447	CO	PRO A	56	40.952	37.502	38.113	1.00	5.03	6	ATOM	500	O	ASP A	61	34.313	45.844	39.065	1.00	6.25	8
ATOM	448	CA	PRO A	56	40.567	39.757	38.732	1.00	5.12	6	ATOM	501	N	LEU A	62	32.228	46.606	39.374	1.00	6.27	7
ATOM	449	CB	PRO A	56	39.282	38.948	39.083	1.00	5.13	6	ATOM	502	CA	LEU A	62	31.732	46.208	38.072	1.00	6.89	6
ATOM	450	CG	PRO A	56	39.914	37.555	39.212	1.00	5.03	6	ATOM	503	CB	LEU A	62	30.242	45.815	38.193	1.00	7.43	6
ATOM	451	C	PRO A	56	41.189	40.335	39.998	1.00	5.03	6	ATOM	504	CG	LEU A	62	29.864	44.704	39.231	1.00	9.12	6
ATOM	452	O	PRO A	56	41.728	39.671	40.862	1.00	5.00	8	ATOM	505	CD1 LEU A	62	28.372	44.443	39.402	1.00	6.08	6	
ATOM	453	N	TYR A	57	41.081	41.640	40.099	1.00	5.00	7	ATOM	506	CD2 LEU A	62	30.514	43.357	38.889	1.00	9.37	6	
ATOM	454	CA	TYR A	57	41.499	42.474	41.207	1.00	5.00	6	ATOM	507	C	LEU A	62	31.934	47.317	37.053	1.00	7.56	6
ATOM	455	CB	TYR A	57	42.042	43.842	40.709	1.00	5.45	6	ATOM	508	O	LEU A	62	31.256	47.422	36.044	1.00	7.76	8
ATOM	456	CG	TYR A	57	42.261	44.833	41.840	1.00	6.29	6	ATOM	509	N	GLY A	63	32.908	48.240	37.209	1.00	7.95	7
ATOM	457	CD1 TYR A	57	43.330	44.634	42.730	1.00	6.86	6	ATOM	510	CA	GLY A	63	33.125	49.350	36.307	1.00	7.98	6	
ATOM	458	CE1 TYR A	57	43.521	45.499	43.810	1.00	7.20	6	ATOM	511	C	GLY A	63	32.529	50.656	36.862	1.00	8.19	6	
ATOM	459	CD2 TYR A	57	41.421	45.913	42.014	1.00	6.52	6	ATOM	512	O	GLY A	63	31.954	51.300	36.064	1.00	7.99	8	
ATOM	460	CE2 TYR A	57	41.634	46.788	43.085	1.00	6.96	6	ATOM	513	N	GLU A	64	32.685	50.974	38.143	1.00	8.78	7	
ATOM	461	C2 TYR A	57	42.669	46.566	43.963	1.00	7.37	6	ATOM	514	CA	GLU A	64	32.154	52.244	38.659	1.00	9.55	6	
ATOM	462	OH	TYR A	57	42.835	47.431	45.036	1.00	7.85	8	ATOM	515	CB	GLU A	64	30.831	52.051	39.398	1.00	10.66	6
ATOM	463	C	TYR A	57	40.372	42.683	42.201	1.00	5.00	8	ATOM	516	CG	GLU A	64	30.916	51.052	40.517	1.00	11.34	6
ATOM	464	O	TYR A	57	40.546	42.347	43.362	1.00	5.00	8	ATOM	517	CD	GLU A	64	29.629	50.986	41.287	1.00	13.83	6
ATOM	465	N	ASP A	58	39.210	43.212	41.826	1.00	5.00	7	ATOM	518	OE1 GLU A	64	29.203	49.959	41.856	1.00	16.12	8	
ATOM	466	CA	ASP A	58	38.134	43.465	42.771	1.00	5.00	6	ATOM	519	OE2 GLU A	64	28.864	51.950	41.397	1.00	15.85	8	
ATOM	467	CB	ASP A	58	38.136	44.990	43.088	1.00	5.00	6	ATOM	520	C	GLU A	64	33.046	52.958	39.664	1.00	9.91	6
ATOM	468	CG	ASP A	58	37.210	45.478	44.152	1.00	5.00	6	ATOM	521	O	GLU A	64	32.691	53.987	40.243	1.00	9.88	8
ATOM	469	OO1 ASP A	58	36.550	44.681	44.829	1.00	5.00	8	ATOM	522	N	PIE A	65	34.212	52.363	39.936	1.00	10.20	7	
ATOM	470	OO2 ASP A	58	36.995	46.702	44.348	1.00	5.00	8	ATOM	523	CA	PIE A	65	35.172	52.891	40.884	1.00	10.39	6	
ATOM	471	C	ASP A	58	36.813	42.974	42.250	1.00	5.00	8	ATOM	524	CB	PIE A	65	35.412	51.981	42.114	1.00	9.02	6
ATOM	472	O	ASP A	58	36.226	43.643	41.379	1.00	5.00	8	ATOM	525	CG	PIE A	65	34.151	51.662	42.878	1.00	8.75	6
ATOM	473	H	LEU A	59	36.258	41.917	42.874	1.00	5.00	7	ATOM	526	CD1 PIE A	65	33.541	50.420	42.829	1.00	7.83	6	
ATOM	474	CA	LEU A	59	34.967	41.399	42.426	1.00	5.00	6	ATOM	527	CD2 PIE A	65	33.508	52.662	43.617	1.00	7.65	6	
ATOM	475	CB	LEU A	59	34.696	40.040	43.128	1.00	6.31	6	ATOM	528	CE1 PIE A	65	32.339	50.164	43.499	1.00	6.31	6	
ATOM	476	CG	LEU A	59	35.782	38.942	42.885	1.00	8.19	6	ATOM	529	CE2 PIE A	65	32.322	52.406	44.296	1.00	6.18	6	
ATOM	477	CD1 LEU A	59	35.479	37.701	43.725	1.00	7.46	6	ATOM	530	CZ	PIE A	65	31.739	51.138	44.248	1.00	5.83	6	

531	ATOH	C	PIIE A	65	36.480	53.123	40.126	1.00	10.75	6
532	ATOH	O	PIIE A	65	36.935	52.381	39.255	1.00	10.67	8
533	ATOH	H	GLN A	66	37.091	54.215	40.584	1.00	11.02	7
534	ATOH	CA	GLN A	66	38.370	54.590	39.964	1.00	11.57	6
535	ATOH	CB	GLN A	66	38.512	56.102	40.168	1.00	15.18	6
536	ATOH	CG	GLN A	66	39.855	56.661	39.832	1.00	20.59	6
537	ATOH	CD	GLN A	66	40.150	56.793	38.363	1.00	24.82	6
538	ATOH	OE1	GLN A	66	39.958	57.812	37.688	1.00	28.38	8
539	ATOH	HE2	GLN A	66	40.716	55.789	37.719	1.00	26.84	7
540	ATOH	C	GLN A	66	39.489	53.768	40.576	1.00	11.54	6
541	ATOH	O	GLN A	66	39.989	54.089	41.699	1.00	11.29	8
542	ATOH	H	GLN A	67	39.870	52.683	39.895	1.00	11.31	7
543	ATOH	CA	GLN A	67	40.915	51.786	40.411	1.00	11.24	6
544	ATOH	CB	GLN A	67	40.390	50.591	41.201	1.00	9.56	6
545	ATOH	CG	GLN A	67	39.353	50.740	42.242	1.00	7.94	6
546	ATOH	CD	GLN A	67	38.970	49.695	43.240	1.00	6.97	6
547	ATOH	OE1	GLN A	67	39.359	49.865	44.405	1.00	7.23	8
548	ATOH	HE2	GLN A	67	38.222	48.659	42.932	1.00	5.00	7
549	ATOH	C	GLN A	67	41.738	51.246	39.242	1.00	11.63	6
550	ATOH	O	GLN A	67	41.158	50.867	38.216	1.00	11.46	8
551	ATOH	H	LYS A	68	43.063	51.149	39.341	1.00	12.10	7
552	ATOH	CA	LYS A	68	43.938	50.664	38.285	1.00	12.61	6
553	ATOH	CB	LYS A	68	43.621	49.280	37.709	1.00	13.06	6
554	ATOH	CG	LYS A	68	43.465	48.179	38.780	1.00	14.46	6
555	ATOH	CD	LYS A	68	44.715	48.024	39.626	1.00	15.01	6
556	ATOH	CE	LYS A	68	44.683	47.225	40.918	1.00	14.26	6
557	ATOH	HZ	LYS A	68	46.062	47.066	41.499	1.00	12.89	7
558	ATOH	C	LYS A	68	43.908	51.710	37.178	1.00	13.39	6
559	ATOH	O	LYS A	68	43.978	51.422	35.955	1.00	14.41	8
560	ATOH	H	GLY A	69	43.764	53.001	37.484	1.00	13.13	7
561	ATOH	CA	GLY A	69	43.739	54.115	36.582	1.00	12.76	6
562	ATOH	CB	GLY A	69	42.535	54.177	35.674	1.00	12.59	6
563	ATOH	O	GLY A	69	42.481	54.975	34.735	1.00	12.74	8
564	ATOH	H	THR A	70	41.497	53.394	35.983	1.00	12.05	7
565	ATOH	CA	THR A	70	40.325	53.375	35.120	1.00	11.09	6
566	ATOH	CB	THR A	70	40.536	52.215	34.122	1.00	9.79	6
567	ATOH	OG1	THR A	70	39.502	52.210	33.117	1.00	10.12	8
568	ATOH	CG2	THR A	70	40.547	50.831	34.773	1.00	9.26	6
569	ATOH	C	THR A	70	39.087	53.169	35.950	1.00	10.63	6
570	ATOH	O	THR A	70	39.115	52.524	36.977	1.00	10.42	8
571	ATOH	H	VAL A	71	37.978	53.737	35.484	1.00	10.18	7
572	ATOH	CA	VAL A	71	36.690	53.549	36.107	1.00	9.77	6
573	ATOH	CB	VAL A	71	34.374	54.448	36.303	1.00	10.20	6
574	ATOH	CG1	VAL A	71	34.374	54.448	36.303	1.00	8.33	6
575	ATOH	CG2	VAL A	71	36.393	55.860	36.919	1.00	9.35	6
576	ATOH	C	VAL A	71	36.093	52.313	35.404	1.00	9.37	6
577	ATOH	O	VAL A	71	35.766	51.299	36.050	1.00	9.39	8
578	ATOH	H	ARG A	72	36.007	52.357	34.089	1.00	8.79	7
579	ATOH	CA	ARG A	72	35.449	51.252	33.344	1.00	8.64	6
580	ATOH	CB	ARG A	72	35.205	51.645	31.846	1.00	7.09	6
581	ATOH	CG	ARG A	72	36.443	51.798	30.962	1.00	6.38	6
582	ATOH	CD	ARG A	72	36.054	51.979	29.499	1.00	6.64	6
583	ATOH	HE	ARG A	72	37.131	52.071	28.536	1.00	6.31	7
584	ATOH	CZ	ARG A	72	38.053	51.266	28.054	1.00	5.00	6
585	ATOH	NH1	ARG A	72	38.926	51.664	27.158	1.00	5.00	7
586	ATOH	NH2	ARG A	72	38.043	50.022	28.506	1.00	5.00	7
587	ATOH	C	ARG A	72	36.316	49.984	33.347	1.00	8.29	6
588	ATOH	O	ARG A	72	37.531	50.080	33.499	1.00	8.41	8
589	ATOH	N	THR A	73	35.700	48.836	33.120	1.00	8.00	7
590	ATOH	CA	THR A	73	36.539	47.632	32.967	1.00	8.12	6
591	ATOH	CB	THR A	73	35.820	46.301	33.270	1.00	6.10	6
592	ATOH	OG1	THR A	73	34.727	46.140	32.317	1.00	5.35	8
593	ATOH	CG2	THR A	73	35.361	46.223	34.730	1.00	5.00	6
594	ATOH	C	THR A	73	36.932	47.628	31.481	1.00	8.12	6
595	ATOH	O	THR A	73	36.630	48.581	30.739	1.00	8.16	8
596	ATOH	H	LYS A	74	37.514	46.575	30.939	1.00	8.08	7
597	ATOH	CA	LYS A	74	37.782	46.496	29.508	1.00	8.07	6
598	ATOH	CB	LYS A	74	38.443	45.122	29.215	1.00	7.37	6
599	ATOH	CG	LYS A	74	38.780	44.864	27.777	1.00	7.51	6
600	ATOH	CD	LYS A	74	39.173	43.465	27.359	1.00	6.71	6
601	ATOH	CE	LYS A	74	39.463	43.461	25.867	1.00	7.86	6
602	ATOH	NZ	LYS A	74	40.043	42.121	25.465	1.00	7.32	7
603	ATOH	C	LYS A	74	36.469	46.596	28.696	1.00	7.96	6
604	ATOH	O	LYS A	74	36.376	47.163	27.598	1.00	7.92	8
605	ATOH	H	TYR A	75	35.375	46.004	29.221	1.00	7.80	7
606	ATOH	CA	TYR A	75	34.113	45.937	28.503	1.00	7.58	6
607	ATOH	CB	TYR A	75	33.400	44.620	29.024	1.00	7.14	6
608	ATOH	CG	TYR A	75	34.311	43.409	28.864	1.00	6.68	6
609	ATOH	CD	TYR A	75	34.853	42.777	29.988	1.00	6.37	6
610	ATOH	CE	TYR A	75	35.716	41.696	29.857	1.00	6.28	6
611	ATOH	CD2	TYR A	75	34.677	42.916	27.589	1.00	6.45	6
612	ATOH	CE2	TYR A	75	35.547	41.855	27.414	1.00	6.14	6
613	ATOH	CZ	TYR A	75	36.039	41.257	28.570	1.00	6.25	6
614	ATOH	OH	TYR A	75	36.913	40.195	28.479	1.00	6.33	8
615	ATOH	C	TYR A	75	33.188	47.141	28.576	1.00	7.81	6
616	ATOH	O	TYR A	75	32.274	47.302	27.713	1.00	7.79	8
617	ATOH	N	GLY A	76	33.355	48.068	29.555	1.00	7.71	7
618	ATOH	CA	GLY A	76	32.468	49.243	29.681	1.00	7.27	6
619	ATOH	C	GLY A	76	32.204	49.486	31.152	1.00	7.13	6
620	ATOH	O	GLY A	76	32.841	48.904	32.048	1.00	6.91	8
621	ATOH	H	THR A	77	31.250	50.356	31.425	1.00	7.24	7
622	ATOH	CA	THR A	77	30.855	50.694	32.813	1.00	7.52	6
623	ATOH	CB	THR A	77	30.386	52.172	32.914	1.00	7.84	6
624	ATOH	OG1	THR A	77	29.223	52.337	32.073	1.00	8.21	8
625	ATOH	CG2	THR A	77	31.378	53.173	32.361	1.00	6.70	6
626	ATOH	C	THR A	77	29.712	49.827	33.304	1.00	7.62	6
627	ATOH	O	THR A	77	28.984	49.118	32.575	1.00	7.39	8
628	ATOH	N	LYS A	78	29.460	49.853	34.611	1.00	7.89	7
629	ATOH	CA	LYS A	78	28.398	49.084	35.247	1.00	8.24	6
630	ATOH	CB	LYS A	78	28.465	49.384	36.759	1.00	8.87	6
631	ATOH	CG	LYS A	78	27.449	48.604	37.551	1.00	11.52	6
632	ATOH	CD	LYS A	78	27.592	49.117	39.004	1.00	13.82	6
633	ATOH	CE	LYS A	78	26.681	48.228	39.824	1.00	15.45	6
634	ATOH	HZ	LYS A	78	26.132	49.000	40.954	1.00	18.28	7
635	ATOH	C	LYS A	78	27.022	49.428	34.735	1.00	8.73	6
636	ATOH	O	LYS A	78	26.165	48.565	34.477	1.00	8.67	8

ATOH	637	H	SER A	79	26.749	50.759	34.578	1.00	9.32	7
ATOH	638	CA	SER A	79	25.401	51.141	34.086	1.00	9.71	6
ATOH	639	CB	SER A	79	25.190	52.607	34.380	1.00	12.14	6
ATOH	640	CG	SER A	79	25.960	53.338	33.488	1.00	15.84	8
ATOH	641	C	SER A	79	25.262	50.703	32.644	1.00	9.79	6
ATOH	642	O	SER A	79	24.142	50.254	32.312	1.00	10.15	8
ATOH	643	H	GLU A	80	26.291	50.655	31.814	1.00	9.56	7
ATOH	644	CA	GLU A	80	26.160	50.128	30.452	1.00	9.39	6
ATOH	645	CB	GLU A	80	27.429	50.452	29.723	1.00	10.04	6
ATOH	646	CG	GLU A	80	27.546	51.928	29.378	1.00	11.54	6
ATOH	647	CD	GLU A	80	28.902	52.167	28.769	1.00	14.36	6
ATOH	648	OE1	GLU A	80	29.881	51.408	28.913	1.00	15.28	8
ATOH	649	OE2	GLU A	80	29.051	53.186	28.075	1.00	18.22	8
ATOH	650	C	GLU A	80	25.853	48.629	30.476	1.00	9.05	6
ATOH	651	O	GLU A	80	25.005	48.179	29.720	1.00	8.72	8
ATOH	652	H	LEU A	81	26.441	47.873	31.394	1.00	9.09	7
ATOH	653	CA	LEU A	81	26.145	46.428	31.534	1.00	9.12	6
ATOH	654	CB	LEU A	81	27.188	45.716	32.385	1.00	8.24	6
ATOH	655	CG	LEU A	81	26.866	44.272	32.843	1.00	8.68	6
ATOH	656	CD	LEU A	81	26.744	43.229	31.738	1.00	7.74	6
ATOH	657	CD2	LEU A	81	27.983	43.841	33.771	1.00	9.60	6
ATOH	658	C	LEU A	81	24.710	46.226	32.053	1.00	9.19	6
ATOH	659	O	LEU A	81	23.952	45.386	31.515	1.00	8.94	8
ATOH	660	H	GLN A	82	24.247	47.005	33.042	1.00	9.33	7
ATOH	661	CA	GLN A	82	22.853	46.834	33.479	1.00	9.81	6
ATOH	662	CB	GLN A	82	22.588	47.739	34.681	1.00	11.55	6
ATOH	663	CG	GLN A	82	23.288	47.105	35.901	1.00	14.03	6
ATOH	664	CD	GLN A	82	23.239	47.993	37.132	1.00	14.62	6
ATOH	665	OE1	GLN A	82	23.497	49.180	36.990	1.00	15.76	8
ATOH	666	NE2	GLN A	82	22.947	47.380	38.266	1.00	14.70	7
ATOH	667	C	GLN A	82	21.878	47.108	32.358	1.00	10.18	6
ATOH	668	O	GLN A	82	20.854	46.455	32.247	1.00	10.30	8
ATOH	669	H	ASP A	83	22.106	48.088	31.501	1.00	10.58	7
ATOH	670	CA	ASP A	83	21.631	48.355	30.317	1.00	11.05	6
ATOH	671	CB	ASP A	83	21.281	49.619	29.514	1.00	15.09	6
ATOH	672	CG	ASP A	83	21.228	50.893	30.246	1.00	18.79	6
ATOH	673	CD1	ASP A	83	20.404	50.950	31.175	1.00	18.59	8
ATOH	674	CD2	ASP A	83	21.832	51.914	29.841	1.00	22.13	8
ATOH	675	C	ASP A	83	21.439	47.203	29.307	1.00	10.81	6
ATOH	676	O	ASP A	83	20.391	46.942	28.751	1.00	11.02	8
ATOH	677	H	ALA A	84	22.562	46.574	29.048	1.00	10.37	7
ATOH	678	CA	ALA A	84	22.630	45.461	28.120	1.00	10.32	6
ATOH	679	CB	ALA A	84	24.057	45.019	27.847	1.00	7.64	6
ATOH	680	CG	ALA A	84	21.758	44.332	28.688	1.00	10.46	6
ATOH	681	O	ALA A	84	20.988	43.692	27.939	1.00	10.32	8
ATOH	682	H	ILE A	85	21.828	44.045	29.995	1.00	10.47	7
ATOH	683	CA	ILE A	85	21.036	42.985	30.642	1.00	10.46	6
ATOH	684	CB	ILE A	85	21.501	42.710	32.116	1.00	9.71	6
ATOH	685	CG2	ILE A	85	20.474	41.875	32.906	1.00	6.40	6
ATOH	686	CD1	ILE A	85	22.921	42.132	32.080	1.00	9.01	6
ATOH	687	CG1	ILE A	85	23.684	42.092	33.399	1.00	10.12	6
ATOH	688	C	ILE A	85	19.543	43.282	30.566	1.00	10.65	6
ATOH	689	O	ILE A	85	18.768	42.340	30.313	1.00	10.41	8
ATOH	690	H	GLY A	86	19.100	44.530	30.757	1.00	11.09	7
ATOH	691	CA	GLY A	86	17.669	44.837	30.621	1.00	11.74	6
ATOH	692	C	GLY A	86	17.181	44.628	29.181	1.00	12.11	6
ATOH	693	O	GLY A	86	16.109	44.068	28.922	1.00	12.28	8
ATOH	694	CA	SER A	87	17.881	45.049	28.130	1.00	12.31	7
ATOH	695	H	SER A	87	17.451	44.776	26.770	1.00	12.79	6
ATOH	696	CB	SER A	87	18.466	45.329	25.735	1.00	13.98	6
ATOH	697	CG	SER A	87	18.420	46.745	26.044	1.00	18.72	8
ATOH	698	C	SER A	87	17.310	43.266	26.465	1.00	12.80	6
ATOH	699	O	SER A	87	16.395	42.812	25.776	1.00	12.92	8
ATOH	700	H	LEU A	88	18.262	42.459	26.958	1.00	12.48	7
ATOH	701	CA	LEU A	88	18.199	41.020	26.764	1.00	12.30	6
ATOH	702	CB	LEU A	88	19.475	40.339	27.265	1.00	11.21	6
ATOH	703	CG	LEU A	88	20.738	40.582	26.420	1.00	10.80	6
ATOH	704	CD1	LEU A	88	21.896	40.048	27.197	1.00	8.96	6
ATOH	705	CD2	LEU A	88	20.566	39.947	25.036	1.00	11.89	6
ATOH	706	C	LEU A	88	16.995	40.443	27.507	1.00	12.23	6
ATOH	707	O	LEU A	88	16.258	39.575	26.993	1.00	12.29	8
ATOH	708	H	ILE A	89	16.784	40.866	28.752	1.00	12.11	7
ATOH	709	CA	ILE A	89	15.679	40.323	29.507	1.00	12.49	6
ATOH	710	CB	ILE A	89	15.713	40.745	30.987	1.00	11.47	6
ATOH	711	CG	ILE A	89	16.594	39.915	31.863	1.00	11.05	6
ATOH	712	CD2	ILE A	89	17.072	38.635	31.719	1.00	11.34	6
ATOH	713	CD1	ILE A	89	17.117	40.353	33.037	1.00	10.31	7
ATOH	714	CE1	ILE A	89	17.865	39.425	33.593	1.00	10.84	6
ATOH	715	NE2	ILE A	89	17.837	38.343	32.823	1.00	11.68	7
ATOH	716	C	ILE A	89	14.378	40.741	28.838	1.00	13.05	6
ATOH	717	O	ILE A	89	13.480	39.910	28.764	1.00	12.72	8
ATOH	718	CA	SER A	90	14.275	41.957	28.285	1.00	13.89	7
ATOH	719	CB	SER A	90	12.957	42.281	27.665	1.00	15.19	6
ATOH	720	CG	SER A	90	12.784	43.796	27.578	1.00	14.96	6
ATOH	721	CG	SER A	90	13.761	44.225	26.638	1.00	19.72	8
ATOH	722	C	SER A	90	12.722	41.472	26.411	1.00	15.94	6
ATOH	723	O	SER A	90	11.612	41.428	25.924	1.00	15.88	8
ATOH	724	H	ARG A	91	13.632	40.675	25.854	1.00	17.41	6
ATOH	725	CA	ARG A	91	13.529	39.799	24.719	1.00	17.41	6
ATOH	726	CB	ARG A	91	14.651	39.930	23.689	1.00	20.09	6
ATOH	727	CG	ARG A	91	14.977	41.595	23.474	1.00	23.93	6
ATOH	728	CD	ARG A	91	14.271	41.859	22.236	1.00	27.09	6
ATOH	729	NE	ARG A	91	14.479	43.230	22.020	1.00	31.65	7
ATOH	730	C2	ARG A	91	15.007	44.382	22.298	1.00	33.62	6
ATOH	731	HI1	ARG A	91	15.835	44.587	23.321	1.00	33.94	7
ATOH	732	HI2	ARG A	91	14.682	45.428	21.512	1.00	34.30	7
ATOH	733	C	ARG A	91	13.594	38.341	25.184	1.00	17.75	6
ATOH	734	O	ARG A	91	13.827	37.473	24.354	1.00	17.92	8
ATOH	735	H	ASN A	92	13.435	38.126	26.487	1.00	17.94	7
ATOH	736	CA	ASN A	92	13.471	36.780	27.044	1.00	17.98	6
ATOH	737	CB	ASN A	92	12.229	35.993	26.546	1.00	24.48	6
ATOH	738	CG	ASN A	92	11.010	36.657	27.191	1.00	29.10	6
ATOH	739	CD1	ASN A	92	10.782	36.615	28.414	1.00	31.71	8
ATOH	740	CD2	ASN A	92	10.235	37.344	26.343	1.00	30.92	7
ATOH	741	C	ASN A	92	14.740	35.989	26.780	1.00	17.40	6
ATOH	742	O	ASN A	92	14.762	34.799	26.423	1.00	17.64	8

743	ATOH	H	VAL A	93	15.886	36.642	26.989	1.00	16.55	7	796	ATOH	O	VAL A	99	34.461	31.987	37.850	1.00	6.46	8
744	ATOH	CA	VAL A	93	17.213	36.038	26.833	1.00	15.28	6	797	ATOH	N	VAL A	100	35.082	34.017	38.489	1.00	6.60	7
745	ATOH	CB	VAL A	93	18.120	36.688	25.785	1.00	12.97	6	798	ATOH	CA	VAL A	100	36.487	33.766	38.594	1.00	6.45	6
746	ATOH	CG1	VAL A	93	19.467	36.021	25.589	1.00	11.55	6	799	ATOH	CB	VAL A	100	37.273	34.786	37.735	1.00	6.89	6
747	ATOH	CG2	VAL A	93	17.378	36.751	24.453	1.00	12.58	6	800	ATOH	CG1	VAL A	100	38.728	34.308	37.697	1.00	6.74	6
748	ATOH	C	VAL A	93	17.771	36.161	28.256	1.00	14.60	6	801	ATOH	CG2	VAL A	100	36.761	34.893	36.314	1.00	6.94	6
749	ATOH	O	VAL A	93	17.736	37.228	28.829	1.00	14.36	8	802	ATOH	C	VAL A	100	36.930	33.803	40.041	1.00	6.61	6
750	ATOH	H	GLN A	94	18.211	35.007	28.742	1.00	13.97	7	803	ATOH	O	VAL A	100	37.306	34.866	40.566	1.00	6.72	8
751	ATOH	CA	GLN A	94	18.792	34.812	30.045	1.00	13.10	6	804	ATOH	N	LEU A	101	36.882	32.651	40.724	1.00	6.41	7
752	ATOH	CB	GLN A	94	18.642	33.375	30.542	1.00	13.62	6	805	ATOH	CA	LEU A	101	37.189	32.537	42.133	1.00	6.10	6
753	ATOH	CG	GLN A	94	17.165	33.203	30.919	1.00	16.17	6	806	ATOH	CB	LEU A	101	36.017	31.716	42.731	1.00	7.20	6
754	ATOH	CD	GLN A	94	17.047	31.828	31.552	1.00	19.51	6	807	ATOH	CG	LEU A	101	34.663	32.479	42.645	1.00	8.90	6
755	ATOH	OE1	GLN A	94	17.710	30.855	31.198	1.00	21.76	8	808	ATOH	CD1	LEU A	101	33.657	31.509	43.300	1.00	9.60	6
756	ATOH	HE2	GLN A	94	16.206	31.683	32.559	1.00	21.21	7	809	ATOH	CD2	LEU A	101	34.726	33.873	43.244	1.00	7.63	6
757	ATOH	C	GLN A	94	20.275	35.223	30.003	1.00	12.28	6	810	ATOH	C	LEU A	101	38.456	31.843	42.579	1.00	5.96	6
758	ATOH	O	GLN A	94	20.882	35.311	28.935	1.00	12.02	8	811	ATOH	O	LEU A	101	38.672	31.740	43.782	1.00	6.02	8
759	ATOH	H	VAL A	95	20.772	35.576	31.218	1.00	11.32	7	812	ATOH	N	ASN A	102	39.260	31.326	41.676	1.00	5.73	7
760	ATOH	CA	VAL A	95	22.144	36.030	31.272	1.00	10.46	6	813	ATOH	CA	ASN A	102	40.471	30.629	42.025	1.00	5.58	6
761	ATOH	CB	VAL A	95	22.215	37.553	31.568	1.00	11.92	6	814	ATOH	CB	ASN A	102	40.963	29.889	40.727	1.00	5.00	6
762	ATOH	CG1	VAL A	95	23.646	38.014	30.411	1.00	12.21	6	815	ATOH	CG	ASN A	102	42.327	29.247	40.912	1.00	5.00	6
763	ATOH	CG2	VAL A	95	22.942	35.269	32.302	1.00	9.65	6	816	ATOH	CG1	ASN A	102	42.309	28.218	41.608	1.00	5.00	8
764	ATOH	C	VAL A	95	21.591	38.367	30.411	1.00	12.21	6	817	ATOH	CD2	ASN A	102	43.493	29.633	40.442	1.00	5.00	7
765	ATOH	O	VAL A	95	22.559	35.259	33.483	1.00	9.73	8	818	ATOH	C	ASN A	102	41.580	31.490	42.620	1.00	5.69	6
766	ATOH	N	TYR A	96	24.034	34.613	31.857	1.00	8.90	7	819	ATOH	O	ASN A	102	42.261	31.045	43.593	1.00	6.11	8
767	ATOH	CA	TYR A	96	24.920	33.882	32.786	1.00	8.34	6	820	ATOH	N	HIS A	103	41.853	32.670	42.103	1.00	5.60	7
768	ATOH	CB	TYR A	96	25.217	32.512	32.267	1.00	8.31	6	821	ATOH	CA	HIS A	103	42.935	33.520	42.506	1.00	5.59	6
769	ATOH	CG	TYR A	96	24.055	31.583	31.987	1.00	8.37	6	822	ATOH	CB	HIS A	103	44.089	33.287	41.487	1.00	6.54	6
770	ATOH	CD1	TYR A	96	24.298	30.500	31.130	1.00	8.46	6	823	ATOH	CG	HIS A	103	43.645	33.442	40.043	1.00	7.70	6
771	ATOH	CE1	TYR A	96	23.255	29.643	30.831	1.00	8.30	6	824	ATOH	CD2	HIS A	103	43.560	34.512	39.230	1.00	6.52	6
772	ATOH	CD2	TYR A	96	22.797	31.752	32.491	1.00	8.19	6	825	ATOH	N	HIS A	103	43.187	32.341	39.282	1.00	9.01	7
773	ATOH	CE2	TYR A	96	21.742	30.928	32.186	1.00	8.05	6	826	ATOH	CE1	HIS A	103	42.794	32.769	38.082	1.00	8.40	6
774	ATOH	CZ	TYR A	96	22.011	29.854	31.363	1.00	7.94	6	827	ATOH	HE2	HIS A	103	42.993	34.113	38.070	1.00	8.31	7
775	ATOH	OH	TYR A	96	21.055	28.940	31.084	1.00	7.64	8	828	ATOH	C	HIS A	103	42.555	34.977	42.419	1.00	5.57	6
776	ATOH	C	TYR A	96	26.218	34.655	33.000	1.00	8.00	6	829	ATOH	O	HIS A	103	41.470	35.229	41.899	1.00	5.20	8
777	ATOH	O	TYR A	96	26.855	35.017	32.005	1.00	7.99	8	830	ATOH	N	LYS A	104	43.438	35.861	42.914	1.00	5.83	7
778	ATOH	H	GLY A	97	26.624	34.919	34.243	1.00	7.85	7	831	ATOH	CA	LYS A	104	43.226	37.313	42.871	1.00	6.01	6
779	ATOH	CA	GLY A	97	27.818	35.671	34.578	1.00	7.64	6	832	ATOH	CB	LYS A	104	42.938	37.971	44.213	1.00	8.00	6
780	ATOH	C	GLY A	97	29.038	34.754	34.756	1.00	7.84	6	833	ATOH	CG	LYS A	104	41.748	37.393	44.978	1.00	8.52	6
781	ATOH	O	GLY A	97	28.950	33.655	35.307	1.00	7.51	8	834	ATOH	CD	LYS A	104	41.373	38.324	46.133	1.00	9.80	6
782	ATOH	HA	ASP A	98	30.194	35.231	34.285	1.00	7.87	7	835	ATOH	CE	LYS A	104	40.973	39.748	45.746	1.00	8.97	6
783	ATOH	CB	ASP A	98	31.455	34.489	34.482	1.00	8.04	6	836	ATOH	NZ	LYS A	104	39.514	39.723	45.383	1.00	8.50	7
784	ATOH	CB	ASP A	98	32.546	34.944	33.523	1.00	7.77	6	837	ATOH	C	LYS A	104	44.489	37.894	42.278	1.00	6.11	6
785	ATOH	CD	ASP A	98	33.916	33.828	33.077	1.00	7.80	6	838	ATOH	O	LYS A	104	45.526	37.321	42.649	1.00	6.50	8
786	ATOH	OE1	ASP A	98	33.791	33.741	31.896	1.00	8.14	8	839	ATOH	N	ALA A	105	44.501	38.896	41.451	1.00	5.96	7
787	ATOH	OE2	ASP A	98	31.868	34.668	35.953	1.00	7.80	6	840	ATOH	CA	ALA A	105	45.660	39.429	40.846	1.00	5.88	6
788	ATOH	O	ASP A	98	31.644	35.739	36.518	1.00	7.83	8	841	ATOH	CB	ALA A	105	45.699	39.063	39.341	1.00	6.37	6
789	ATOH	N	VAL A	99	32.333	33.601	36.602	1.00	7.25	6	842	ATOH	C	ALA A	105	45.785	40.943	41.031	1.00	6.37	6
790	ATOH	CA	VAL A	99	32.708	33.576	38.035	1.00	7.67	7	843	ATOH	O	ALA A	105	44.741	41.578	41.199	1.00	6.24	8
791	ATOH	CB	VAL A	99	31.742	32.652	38.791	1.00	8.70	6	844	ATOH	N	GLY A	106	46.958	41.584	41.044	1.00	6.40	7
792	ATOH	CG	VAL A	99	32.193	32.306	40.195	1.00	8.70	6	845	ATOH	CA	GLY A	106	47.040	43.001	41.190	1.00	6.60	6
793	ATOH	CG1	VAL A	99	31.943	32.362	38.885	1.00	9.79	6	846	ATOH	C	GLY A	106	47.006	43.611	42.573	1.00	7.01	6
794	ATOH	CG2	VAL A	99	30.366	33.362	38.885	1.00	9.79	6	847	ATOH	O	GLY A	106	46.524	44.736	42.659	1.00	6.76	8
795	ATOH	C	VAL A	99	34.155	33.123	38.148	1.00	6.81	6	848	ATOH	N	ALA A	107	47.489	42.945	43.637	1.00	7.49	7

ATOH	849	CA	ALA A 107	47.462	43.434	44.979	1.00	7.87	6
ATOH	850	CB	ALA A 107	48.271	42.572	45.920	1.00	5.59	6
ATOH	851	C	ALA A 107	48.055	44.842	44.970	1.00	8.71	6
ATOH	852	O	ALA A 107	48.875	45.204	44.120	1.00	8.95	8
ATOH	853	H	ASP A 108	47.647	45.649	45.934	1.00	9.17	7
ATOH	854	CA	ASP A 108	48.106	47.011	46.130	1.00	9.77	6
ATOH	855	CB	ASP A 108	47.118	47.666	47.155	1.00	10.59	6
ATOH	856	CG	ASP A 108	45.718	47.703	46.582	1.00	10.42	6
ATOH	857	OO1	ASP A 108	44.685	47.094	46.851	1.00	10.41	8
ATOH	858	OO2	ASP A 108	45.580	48.455	45.604	1.00	12.47	8
ATOH	859	C	ASP A 108	49.530	47.044	46.683	1.00	10.18	6
ATOH	860	O	ASP A 108	50.281	48.011	46.478	1.00	10.34	8
ATOH	861	H	ALA A 109	49.958	46.023	47.436	1.00	10.17	7
ATOH	862	CA	ALA A 109	51.273	45.970	48.023	1.00	10.21	6
ATOH	863	CB	ALA A 109	51.271	46.787	49.322	1.00	10.14	6
ATOH	864	C	ALA A 109	51.669	44.553	48.398	1.00	10.56	6
ATOH	865	O	ALA A 109	50.836	43.629	48.473	1.00	10.49	8
ATOH	866	H	THR A 110	52.966	44.438	48.710	1.00	10.81	7
ATOH	867	CA	THR A 110	53.504	43.168	49.132	1.00	11.01	6
ATOH	868	CB	THR A 110	54.958	42.954	48.705	1.00	11.26	6
ATOH	869	CG1	THR A 110	55.741	43.988	49.294	1.00	11.79	8
ATOH	870	CG2	THR A 110	55.196	43.055	47.209	1.00	11.23	6
ATOH	871	C	THR A 110	53.445	43.091	50.643	1.00	11.37	6
ATOH	872	O	THR A 110	53.349	44.102	51.351	1.00	11.33	8
ATOH	873	H	GLU A 111	53.477	41.851	51.165	1.00	11.70	7
ATOH	874	CA	GLU A 111	53.527	41.504	52.566	1.00	11.89	6
ATOH	875	CB	GLU A 111	52.223	40.870	53.035	1.00	10.98	6
ATOH	876	CG	GLU A 111	51.153	41.995	53.103	1.00	13.17	6
ATOH	877	CD	GLU A 111	49.812	41.428	53.483	1.00	14.55	8
ATOH	878	OE1	GLU A 111	49.365	40.456	52.823	1.00	14.72	6
ATOH	879	OE2	GLU A 111	49.218	41.958	54.436	1.00	15.89	8
ATOH	880	C	GLU A 111	54.697	40.516	52.799	1.00	12.41	6
ATOH	881	O	GLU A 111	55.011	39.715	51.878	1.00	12.71	7
ATOH	882	H	ASP A 112	55.284	40.485	53.981	1.00	12.22	8
ATOH	883	CA	ASP A 112	56.344	39.543	54.283	1.00	13.23	6
ATOH	884	CB	ASP A 112	57.290	39.993	55.380	1.00	18.18	6
ATOH	885	CG	ASP A 112	58.008	41.297	55.120	1.00	21.75	6
ATOH	886	OO1	ASP A 112	58.435	41.747	54.039	1.00	23.40	8
ATOH	887	OO2	ASP A 112	58.189	42.024	56.128	1.00	24.60	8
ATOH	888	C	ASP A 112	55.666	38.250	54.730	1.00	13.29	6
ATOH	889	O	ASP A 112	54.802	38.272	55.608	1.00	13.60	8
ATOH	890	H	VAL A 113	56.015	37.098	54.155	1.00	13.02	7
ATOH	891	CA	VAL A 113	55.381	35.819	54.410	1.00	12.74	6
ATOH	892	CB	VAL A 113	54.466	35.495	53.205	1.00	13.86	6
ATOH	893	CG1	VAL A 113	53.650	34.192	53.418	1.00	14.55	6
ATOH	894	CG2	VAL A 113	53.423	36.541	52.806	1.00	13.68	6
ATOH	895	C	VAL A 113	56.407	34.721	54.511	1.00	12.52	6
ATOH	896	O	VAL A 113	57.412	34.748	53.765	1.00	12.66	8
ATOH	897	H	THR A 114	56.238	33.728	55.355	1.00	12.21	7
ATOH	898	CA	THR A 114	57.167	32.595	55.443	1.00	11.87	6
ATOH	899	CB	THR A 114	57.212	31.941	56.800	1.00	12.24	6
ATOH	900	CG1	THR A 114	57.602	32.955	57.741	1.00	14.04	8
ATOH	901	CG2	THR A 114	58.195	30.781	56.909	1.00	10.63	6
ATOH	902	C	THR A 114	56.563	31.547	54.495	1.00	11.69	6
ATOH	903	O	THR A 114	55.355	31.265	54.457	1.00	11.32	8
ATOH	904	N	ALA A 115	57.429	31.042	53.643	1.00	11.64	7
ATOH	905	CA	ALA A 115	57.024	30.048	52.638	1.00	11.55	6
ATOH	906	CB	ALA A 115	56.825	30.894	51.357	1.00	10.80	6
ATOH	907	C	ALA A 115	58.039	28.947	52.343	1.00	11.45	6
ATOH	908	O	ALA A 115	59.215	29.073	52.688	1.00	11.41	8
ATOH	909	H	VAL A 116	57.641	27.868	51.657	1.00	11.33	7
ATOH	910	CA	VAL A 116	58.513	26.814	51.184	1.00	11.10	6
ATOH	911	CB	VAL A 116	58.338	25.436	51.815	1.00	12.01	6
ATOH	912	CG1	VAL A 116	58.978	25.449	53.208	1.00	12.23	6
ATOH	913	CG2	VAL A 116	56.882	24.978	51.873	1.00	11.15	6
ATOH	914	C	VAL A 116	58.250	26.642	49.656	1.00	10.95	6
ATOH	915	O	VAL A 116	57.100	26.960	49.240	1.00	11.03	8
ATOH	916	H	GLU A 117	59.187	26.205	48.856	1.00	10.29	7
ATOH	917	CA	GLU A 117	58.932	25.898	47.465	1.00	11.06	6
ATOH	918	CB	GLU A 117	60.201	25.861	46.625	1.00	11.90	6
ATOH	919	CG	GLU A 117	60.905	27.201	46.773	1.00	14.30	6
ATOH	920	CD	GLU A 117	62.245	27.143	46.070	1.00	16.13	6
ATOH	921	OE1	GLU A 117	62.515	26.342	45.175	1.00	16.80	8
ATOH	922	OE2	GLU A 117	63.067	28.004	46.366	1.00	17.32	8
ATOH	923	C	GLU A 117	58.354	24.480	47.369	1.00	9.67	6
ATOH	924	O	GLU A 117	58.596	23.656	48.258	1.00	9.47	8
ATOH	925	N	VAL A 118	57.623	24.157	46.316	1.00	9.40	7
ATOH	926	CA	VAL A 118	56.987	22.802	46.152	1.00	10.25	6
ATOH	927	CB	VAL A 118	55.556	23.243	46.543	1.00	10.55	6
ATOH	928	CG1	VAL A 118	54.529	23.164	45.421	1.00	9.52	6
ATOH	929	CG2	VAL A 118	55.061	22.664	47.855	1.00	10.49	6
ATOH	930	C	VAL A 118	57.360	22.305	44.765	1.00	9.31	6
ATOH	931	O	VAL A 118	57.660	23.097	43.823	1.00	9.23	8
ATOH	932	N	ASN A 119	57.381	20.998	44.492	1.00	8.84	7
ATOH	933	CA	ASN A 119	57.701	20.403	43.206	1.00	8.20	6
ATOH	934	CB	ASN A 119	57.911	18.914	43.534	1.00	7.82	6
ATOH	935	CG	ASN A 119	58.248	18.097	42.289	1.00	8.10	6
ATOH	936	OO1	ASN A 119	58.084	18.636	41.177	1.00	7.16	8
ATOH	937	OO2	ASN A 119	58.706	16.848	42.386	1.00	6.98	7
ATOH	938	C	ASN A 119	56.553	20.692	42.242	1.00	7.98	6
ATOH	939	O	ASN A 119	55.382	20.414	42.482	1.00	7.64	8
ATOH	940	N	PRO A 120	56.833	21.326	41.094	1.00	8.04	7
ATOH	941	CD	PRO A 120	58.207	21.735	40.728	1.00	8.00	6
ATOH	942	CO	PRO A 120	55.849	21.704	40.088	1.00	8.27	6
ATOH	943	CB	PRO A 120	56.609	22.404	38.938	1.00	8.21	6
ATOH	944	CG	PRO A 120	57.980	22.618	39.530	1.00	8.16	6
ATOH	945	C	PRO A 120	55.032	20.526	39.601	1.00	8.65	6
ATOH	946	O	PRO A 120	53.858	20.633	39.275	1.00	8.69	8
ATOH	947	H	ALA A 121	55.648	19.337	39.540	1.00	9.00	7
ATOH	948	CA	ALA A 121	54.977	18.104	39.122	1.00	9.39	6
ATOH	949	CB	ALA A 121	55.976	17.215	38.324	1.00	9.49	6
ATOH	950	C	ALA A 121	54.374	17.315	40.267	1.00	9.46	6
ATOH	951	O	ALA A 121	53.644	16.327	40.066	1.00	9.60	8
ATOH	952	H	ASN A 122	54.624	17.656	41.537	1.00	9.45	7
ATOH	953	CA	ASN A 122	54.040	16.971	42.679	1.00	9.32	6
ATOH	954	CB	ASN A 122	54.881	15.802	43.207	1.00	10.30	6

ATOM	955	CG	ASH A 122	54.009	15.047	44.180	1.00	13.39	6	ATOM	1008	C	SER A 128	62.620	23.784	51.617	1.00	18.11	6
ATOM	956	001	ASH A 122	53.085	15.591	44.786	1.00	13.50	8	ATOM	1009	O	SER A 128	61.642	23.256	52.161	1.00	17.96	8
ATOM	957	W02	ASH A 122	54.211	13.733	44.357	1.00	16.10	7	ATOM	1010	H	GLU A 129	63.523	24.444	52.326	1.00	18.90	7
ATOM	958	C	ASH A 122	53.936	18.050	43.742	1.00	9.22	6	ATOM	1011	CA	GLU A 129	63.395	24.747	53.735	1.00	19.85	6
ATOM	959	O	ASH A 122	54.881	18.130	44.566	1.00	9.02	8	ATOM	1012	CB	GLU A 129	64.718	25.038	54.440	1.00	27.78	6
ATOM	960	H	ARG A 123	52.869	18.855	43.722	1.00	9.27	7	ATOM	1013	CG	GLU A 129	64.794	24.360	55.817	1.00	35.30	6
ATOM	961	CA	ARG A 123	52.764	19.983	44.684	1.00	9.23	6	ATOM	1014	CD	GLU A 129	65.311	22.937	55.587	1.00	40.42	6
ATOM	962	CB	ARG A 123	51.675	20.969	44.227	1.00	7.86	6	ATOM	1015	OE1	GLU A 129	66.375	22.846	54.891	1.00	43.75	8
ATOM	963	CD	ARG A 123	52.067	21.746	42.991	1.00	6.67	6	ATOM	1016	OE2	GLU A 129	64.637	21.983	56.055	1.00	42.88	8
ATOM	964	CG	ARG A 123	51.511	21.080	41.764	1.00	6.95	6	ATOM	1017	C	GLU A 129	62.566	26.060	53.737	1.00	19.69	6
ATOM	965	NE	ARG A 123	51.759	21.959	40.604	1.00	9.73	7	ATOM	1018	O	GLU A 129	62.573	26.773	52.713	1.00	19.50	8
ATOM	966	CZ	ARG A 123	50.906	22.937	40.275	1.00	10.25	6	ATOM	1019	H	GLU A 130	61.925	26.390	54.849	1.00	19.52	7
ATOM	967	HH1	ARG A 123	49.828	23.054	41.044	1.00	9.79	7	ATOM	1020	CA	GLU A 130	61.150	27.612	54.769	1.00	19.43	6
ATOM	968	HH2	ARG A 123	51.000	23.793	39.273	1.00	10.20	7	ATOM	1021	CG	GLU A 130	60.090	27.530	55.847	1.00	23.57	6
ATOM	969	C	ARG A 123	52.593	19.557	46.158	1.00	9.23	6	ATOM	1022	CG	GLU A 130	60.633	27.773	57.215	1.00	26.39	6
ATOM	970	O	ARG A 123	52.622	20.374	47.085	1.00	8.71	8	ATOM	1023	CD	GLU A 130	59.542	27.368	58.202	1.00	29.94	6
ATOM	971	H	ASH A 124	52.408	18.256	46.379	1.00	9.56	7	ATOM	1024	OE1	GLU A 130	59.493	28.140	59.202	1.00	33.34	8
ATOM	972	CA	ASH A 124	52.351	17.706	47.712	1.00	10.31	6	ATOM	1025	OE2	GLU A 130	58.779	26.388	58.051	1.00	30.50	8
ATOM	973	CB	ASH A 124	51.742	16.299	47.800	1.00	11.34	6	ATOM	1026	C	GLU A 130	61.988	28.851	54.837	1.00	18.97	6
ATOM	974	CG	ASH A 124	50.275	16.347	47.455	1.00	14.21	6	ATOM	1027	O	GLU A 130	63.023	28.894	55.454	1.00	19.04	8
ATOM	975	001	ASH A 124	49.565	17.271	47.867	1.00	14.26	8	ATOM	1028	N	TYR A 131	61.506	29.854	54.117	1.00	18.45	7
ATOM	976	W02	ASH A 124	49.887	15.391	46.590	1.00	16.51	7	ATOM	1029	CA	TYR A 131	62.186	31.164	54.098	1.00	17.87	6
ATOM	977	C	ASH A 124	53.796	17.564	48.243	1.00	10.74	6	ATOM	1030	CB	TYR A 131	63.336	31.254	53.126	1.00	18.14	6
ATOM	978	O	ASN A 124	53.926	17.342	49.439	1.00	10.85	8	ATOM	1031	CG	TYR A 131	63.123	31.022	51.656	1.00	18.56	6
ATOM	979	H	GLN A 125	54.872	17.660	47.433	1.00	10.96	7	ATOM	1032	CD1	TYR A 131	63.015	32.108	50.786	1.00	18.80	6
ATOM	980	CA	GLN A 125	56.223	17.549	47.925	1.00	11.21	6	ATOM	1033	CD1	TYR A 131	62.837	31.915	49.415	1.00	18.78	6
ATOM	981	CB	GLN A 125	57.169	16.823	46.919	1.00	9.50	6	ATOM	1034	CD2	TYR A 131	63.053	29.741	51.125	1.00	18.56	6
ATOM	982	CG	GLN A 125	58.582	16.600	47.498	1.00	8.17	6	ATOM	1035	CE2	TYR A 131	62.856	29.566	49.772	1.00	18.73	6
ATOM	984	OE1	GLN A 125	59.546	16.199	46.402	1.00	8.01	6	ATOM	1036	CZ	TYR A 131	62.753	30.638	48.908	1.00	18.74	6
ATOM	985	NE2	GLN A 125	59.184	16.310	45.207	1.00	6.56	8	ATOM	1037	OH	TYR A 131	62.618	30.432	47.547	1.00	18.62	8
ATOM	986	C	GLN A 125	60.762	15.784	46.738	1.00	6.20	7	ATOM	1038	C	TYR A 131	61.150	32.287	53.841	1.00	17.13	6
ATOM	987	O	GLN A 125	56.871	18.915	48.156	1.00	11.48	6	ATOM	1039	O	TYR A 131	59.992	32.053	53.530	1.00	16.72	8
ATOM	988	H	GLU A 126	57.345	19.217	49.360	1.00	11.44	8	ATOM	1040	N	GLN A 132	61.601	33.503	54.011	1.00	16.51	7
ATOM	989	CA	GLU A 126	58.053	20.468	49.610	1.00	12.46	6	ATOM	1041	CA	GLN A 132	60.855	34.718	53.865	1.00	16.10	6
ATOM	990	CB	GLU A 126	58.042	20.856	51.115	1.00	11.31	6	ATOM	1042	CB	GLN A 132	61.459	35.882	54.723	1.00	22.79	6
ATOM	991	CG	GLU A 126	56.589	20.799	51.582	1.00	12.45	6	ATOM	1043	CG	GLN A 132	60.607	35.969	55.997	1.00	29.13	6
ATOM	992	CD	GLU A 126	56.371	21.288	52.993	1.00	13.36	6	ATOM	1044	CD	GLN A 132	61.036	34.850	56.938	1.00	33.56	6
ATOM	993	OE1	GLU A 126	57.329	21.471	53.748	1.00	13.22	8	ATOM	1045	OE1	GLN A 132	62.246	34.859	57.308	1.00	37.13	8
ATOM	994	OE2	GLU A 126	55.214	21.519	53.374	1.00	14.72	8	ATOM	1046	NE2	GLN A 132	60.138	33.934	57.337	1.00	34.32	7
ATOM	995	C	GLU A 126	59.513	20.293	49.195	1.00	13.18	6	ATOM	1047	C	GLN A 132	60.810	35.316	52.481	1.00	15.05	6
ATOM	996	O	GLU A 126	60.198	19.292	49.513	1.00	12.98	8	ATOM	1048	O	GLN A 132	61.881	35.620	51.931	1.00	15.27	8
ATOM	997	H	THR A 127	60.045	21.216	48.430	1.00	14.11	7	ATOM	1049	N	ILE A 133	59.589	35.505	51.972	1.00	12.62	6
ATOM	998	CA	THR A 127	61.407	21.048	47.954	1.00	15.19	6	ATOM	1050	CA	ILE A 133	59.481	36.102	50.631	1.00	13.86	7
ATOM	999	CB	THR A 127	61.487	21.193	46.420	1.00	14.68	6	ATOM	1051	CB	ILE A 133	58.828	35.111	49.616	1.00	11.38	6
ATOM	1000	CG1	THR A 127	60.732	22.349	46.071	1.00	15.49	8	ATOM	1052	CG2	ILE A 133	59.610	33.787	49.469	1.00	9.01	6
ATOM	1001	CG2	THR A 127	60.902	19.957	45.774	1.00	13.94	6	ATOM	1053	CG1	ILE A 133	57.374	34.744	49.978	1.00	11.33	6
ATOM	1002	C	THR A 127	62.377	21.993	48.614	1.00	16.26	6	ATOM	1054	CD1	ILE A 133	56.601	33.908	48.958	1.00	11.24	6
ATOM	1003	O	THR A 127	63.552	21.851	48.283	1.00	16.67	8	ATOM	1055	C	ILE A 133	58.652	37.381	50.761	1.00	11.82	6
ATOM	1004	N	SER A 128	62.015	22.892	49.503	1.00	16.75	7	ATOM	1056	O	ILE A 133	58.026	37.593	51.790	1.00	11.18	8
ATOM	1005	CA	SER A 128	63.000	23.747	50.125	1.00	17.24	6	ATOM	1057	H	LYS A 134	58.611	38.192	49.709	1.00	11.45	7
ATOM	1006	CB	SER A 128	63.016	25.141	49.511	1.00	15.04	6	ATOM	1058	CA	LYS A 134	57.737	39.379	49.674	1.00	11.11	6
ATOM	1007	OG	SER A 128	61.873	25.859	49.965	1.00	13.39	8	ATOM	1059	CB	LYS A 134	58.443	40.661	49.331	1.00	12.71	6
										ATOM	1060	CG	LYS A 134	59.019	41.223	50.642	1.00	15.80	6

1061	ATOH	CD	LYS A 134	59.998	42.325	50.294	1.00	19.11	6
1062	ATOH	CE	LYS A 134	59.652	43.476	51.253	1.00	22.58	6
1063	ATOH	HZ	LYS A 134	59.863	42.966	52.656	1.00	24.21	7
1064	ATOH	C	LYS A 134	56.683	39.046	48.618	1.00	10.75	6
1065	ATOH	O	LYS A 134	57.075	38.997	47.439	1.00	10.72	8
1066	ATOH	H	ALA A 135	55.444	38.754	48.993	1.00	10.26	7
1067	ATOH	CA	ALA A 135	54.411	38.356	48.046	1.00	9.82	6
1068	ATOH	CB	ALA A 135	53.713	37.071	48.552	1.00	8.45	6
1069	ATOH	C	ALA A 135	53.360	39.428	47.848	1.00	9.62	6
1070	ATOH	O	ALA A 135	53.052	40.158	48.834	1.00	9.91	8
1071	ATOH	H	TRP A 136	52.718	39.492	46.672	1.00	9.28	7
1072	ATOH	CA	TRP A 136	51.676	40.473	46.354	1.00	8.76	6
1073	ATOH	CB	TRP A 136	51.683	40.690	44.846	1.00	9.45	6
1074	ATOH	CG	TRP A 136	52.918	41.438	44.430	1.00	12.78	6
1075	ATOH	CD	TRP A 136	53.068	42.881	44.426	1.00	13.09	6
1076	ATOH	CE	TRP A 136	54.343	43.162	43.888	1.00	14.31	6
1077	ATOH	CE	TRP A 136	52.224	43.924	44.799	1.00	11.71	6
1078	ATOH	CE	TRP A 136	54.098	40.924	43.934	1.00	13.83	6
1079	ATOH	CE	TRP A 136	54.954	41.951	43.599	1.00	15.49	7
1080	ATOH	CE	TRP A 136	54.846	44.456	43.772	1.00	14.17	6
1081	ATOH	CE	TRP A 136	52.680	45.213	44.627	1.00	12.36	6
1082	ATOH	CE	TRP A 136	53.971	45.463	44.144	1.00	13.78	6
1083	ATOH	C	TRP A 136	50.338	39.995	46.811	1.00	8.40	6
1084	ATOH	O	TRP A 136	49.535	39.452	46.066	1.00	8.39	8
1085	ATOH	H	THR A 137	50.028	40.192	48.086	1.00	8.12	7
1086	ATOH	CB	THR A 137	49.275	39.707	48.761	1.00	7.75	6
1087	ATOH	CB	THR A 137	48.844	38.704	49.884	1.00	7.93	6
1088	ATOH	OG	THR A 137	50.351	39.218	50.701	1.00	8.77	8
1089	ATOH	CG	THR A 137	49.847	37.387	49.327	1.00	8.10	6
1090	ATOH	C	THR A 137	48.040	40.772	49.490	1.00	7.59	6
1091	ATOH	O	THR A 137	47.063	40.370	50.112	1.00	7.09	8
1092	ATOH	H	ASP A 138	48.425	42.026	49.486	1.00	7.55	7
1093	ATOH	CA	ASP A 138	47.680	43.038	50.221	1.00	7.91	6
1094	ATOH	CB	ASP A 138	48.667	44.060	50.793	1.00	10.34	6
1095	ATOH	CG	ASP A 138	48.054	45.085	51.742	1.00	14.50	6
1096	ATOH	OD	ASP A 138	46.820	45.294	51.881	1.00	14.46	8
1097	ATOH	O	ASP A 138	48.845	45.781	52.416	1.00	16.18	8
1098	ATOH	C	ASP A 138	46.627	43.671	49.316	1.00	8.01	6
1099	ATOH	O	ASP A 138	47.039	44.379	48.405	1.00	7.97	8
1100	ATOH	H	PIE A 140	45.334	43.427	49.520	1.00	8.44	7
1101	ATOH	CA	PIE A 140	44.298	44.016	48.652	1.00	9.00	6
1102	ATOH	CB	PIE A 140	43.394	43.011	47.964	1.00	7.03	6
1103	ATOH	CG	PIE A 140	44.078	42.176	46.892	1.00	8.72	6
1104	ATOH	CD	PIE A 140	44.948	41.138	47.287	1.00	7.30	6
1105	ATOH	CE	PIE A 140	43.835	42.398	45.538	1.00	7.95	6
1106	ATOH	CE	PIE A 140	45.600	40.359	46.350	1.00	8.84	6
1107	ATOH	CE	PIE A 140	44.469	41.605	44.591	1.00	8.85	6
1108	ATOH	C	PIE A 140	45.335	40.593	44.979	1.00	9.11	6
1109	ATOH	O	PIE A 140	43.461	44.987	49.487	1.00	9.73	6
1110	ATOH	H	ARG A 140	42.707	44.536	50.343	1.00	9.71	8
1111	ATOH	N	ARG A 140	43.599	46.294	49.178	1.00	10.52	7
1112	ATOH	CA	ARG A 140	42.823	47.246	49.985	1.00	11.46	6
1113	ATOH	CB	ARG A 140	43.647	48.263	50.745	1.00	17.79	6
1114	ATOH	CG	ARG A 140	45.059	48.594	50.380	1.00	22.69	6
1115	ATOH	CD	ARG A 140	45.796	48.583	51.753	1.00	27.78	6
1116	ATOH	NE	ARG A 140	47.197	48.785	51.626	1.00	32.35	7
1117	ATOH	CZ	ARG A 140	48.476	48.985	51.487	1.00	34.38	6
1118	ATOH	NH1	ARG A 140	48.873	49.714	50.421	1.00	34.62	7
1119	ATOH	NH2	ARG A 140	49.440	48.518	52.329	1.00	34.86	7
1120	ATOH	C	ARG A 140	41.766	48.037	49.205	1.00	11.28	6
1121	ATOH	O	ARG A 140	40.965	48.699	49.916	1.00	11.54	8
1122	ATOH	N	PIE A 141	41.672	47.993	47.908	1.00	10.83	7
1123	ATOH	CA	PIE A 141	40.554	48.658	47.231	1.00	10.94	6
1124	ATOH	CB	PIE A 141	39.237	47.897	47.618	1.00	8.15	6
1125	ATOH	CG	PIE A 141	39.346	46.381	47.561	1.00	6.78	6
1126	ATOH	CD	PIE A 141	39.041	45.616	48.673	1.00	5.88	6
1127	ATOH	CE	PIE A 141	39.793	45.725	46.453	1.00	5.72	6
1128	ATOH	CE	PIE A 141	39.150	44.225	48.627	1.00	6.27	6
1129	ATOH	CE	PIE A 141	39.930	44.318	46.407	1.00	5.00	6
1130	ATOH	CZ	PIE A 141	39.607	43.584	47.478	1.00	5.00	6
1131	ATOH	C	PIE A 141	40.372	50.134	47.543	1.00	11.05	6
1132	ATOH	O	PIE A 141	39.377	50.553	48.103	1.00	10.80	8
1133	ATOH	N	PRO A 142	41.402	50.934	47.254	1.00	11.32	7
1134	ATOH	CD	PRO A 142	42.645	50.440	46.634	1.00	11.43	6
1135	ATOH	CA	PRO A 142	41.462	52.384	47.515	1.00	11.27	6
1136	ATOH	CB	PRO A 142	42.900	52.829	47.190	1.00	11.50	6
1137	ATOH	CG	PRO A 142	43.300	51.728	46.191	1.00	11.68	6
1138	ATOH	C	PRO A 142	40.424	53.179	46.766	1.00	11.03	6
1139	ATOH	O	PRO A 142	39.933	54.100	47.431	1.00	11.24	8
1140	ATOH	N	GLY A 143	39.984	52.964	45.545	1.00	10.61	7
1141	ATOH	CA	GLY A 143	38.950	53.703	44.905	1.00	10.26	6
1142	ATOH	C	GLY A 143	37.544	53.272	45.330	1.00	10.29	6
1143	ATOH	O	GLY A 143	36.578	54.011	45.134	1.00	10.11	8
1144	ATOH	H	ARG A 144	37.337	52.102	45.941	1.00	10.41	7
1145	ATOH	CA	ARG A 144	36.034	51.630	46.365	1.00	10.66	6
1146	ATOH	CB	ARG A 144	35.855	50.122	46.066	1.00	6.45	6
1147	ATOH	CG	ARG A 144	34.545	49.572	46.609	1.00	6.10	6
1148	ATOH	CD	ARG A 144	34.074	48.222	46.139	1.00	7.45	6
1149	ATOH	NE	ARG A 144	35.003	47.110	46.397	1.00	6.59	6
1150	ATOH	CZ	ARG A 144	35.062	46.377	47.500	1.00	7.53	6
1151	ATOH	NH1	ARG A 144	35.983	45.402	47.626	1.00	8.54	7
1152	ATOH	NH2	ARG A 144	36.219	46.599	48.511	1.00	6.60	7
1153	ATOH	C	ARG A 144	35.736	51.908	47.869	1.00	11.31	6
1154	ATOH	O	ARG A 144	34.643	52.176	48.348	1.00	11.05	8
1155	ATOH	H	GLY A 145	36.813	51.804	48.658	1.00	11.78	7
1156	ATOH	CA	GLY A 145	36.758	51.954	50.104	1.00	12.35	6
1157	ATOH	C	GLY A 145	35.922	50.757	50.584	1.00	12.97	6
1158	ATOH	O	GLY A 145	36.169	49.601	50.164	1.00	13.33	8
1159	ATOH	N	ASN A 146	34.906	51.057	51.416	1.00	12.95	7
1160	ATOH	CA	ASN A 146	34.070	49.991	51.970	1.00	12.83	6
1161	ATOH	CB	ASN A 146	33.889	50.195	53.493	1.00	15.58	6
1162	ATOH	CG	ASN A 146	35.151	49.936	54.288	1.00	19.40	6
1163	ATOH	OD	ASN A 146	36.065	49.159	53.989	1.00	20.79	8
1164	ATOH	NH2	ASN A 146	35.264	50.678	55.410	1.00	20.44	7
1165	ATOH	C	ASN A 146	32.689	49.855	51.336	1.00	12.13	6
1166	ATOH	O	ASN A 146	31.905	49.168	52.002	1.00	12.08	8

ATOM	1167	H	THR A 147	32.491	50.456	50.175	1.00	11.60	7	ATOM	1220	H	TRP A 153	41.841	41.875	51.926	1.00	8.13	7
ATOM	1168	CA	THR A 147	31.200	50.351	49.487	1.00	11.26	6	ATOM	1221	CA	TRP A 153	42.585	40.644	51.805	1.00	7.85	6
ATOM	1169	CB	THR A 147	31.164	51.128	48.161	1.00	11.45	6	ATOM	1222	CB	TRP A 153	42.567	40.241	50.293	1.00	6.88	6
ATOM	1170	CG1	THR A 147	31.709	52.445	48.360	1.00	12.12	8	ATOM	1223	CG	TRP A 153	41.174	39.851	49.872	1.00	6.70	6
ATOM	1171	CG2	THR A 147	29.782	51.325	47.548	1.00	9.27	6	ATOM	1224	CG2	TRP A 153	40.681	38.522	49.679	1.00	6.38	6
ATOM	1172	C	THR A 147	30.895	48.884	49.247	1.00	11.00	6	ATOM	1225	CE2	TRP A 153	39.330	38.637	49.270	1.00	7.85	6
ATOM	1173	O	THR A 147	31.757	48.136	48.721	1.00	11.07	8	ATOM	1226	CE3	TRP A 153	41.225	37.236	49.779	1.00	6.59	6
ATOM	1174	H	TYR A 148	29.718	48.430	49.662	1.00	10.51	7	ATOM	1227	CD1	TRP A 153	40.139	40.695	49.600	1.00	6.77	6
ATOM	1175	CA	TYR A 148	29.245	47.066	49.538	1.00	10.35	6	ATOM	1228	HE1	TRP A 153	39.018	39.986	49.233	1.00	6.86	7
ATOM	1176	CB	TYR A 148	29.308	46.455	48.113	1.00	10.34	6	ATOM	1229	CZ2	TRP A 153	38.542	37.504	48.986	1.00	7.93	6
ATOM	1177	CG	TYR A 148	28.798	47.326	46.967	1.00	9.97	6	ATOM	1230	CZ3	TRP A 153	40.477	36.113	49.452	1.00	7.12	6
ATOM	1178	CD1	TYR A 148	29.649	47.666	45.916	1.00	9.49	6	ATOM	1231	CH2	TRP A 153	39.128	36.250	49.081	1.00	8.55	6
ATOM	1179	CE1	TYR A 148	29.177	48.430	44.845	1.00	9.11	6	ATOM	1232	C	TRP A 153	44.014	40.738	52.256	1.00	7.70	6
ATOM	1180	CD2	TYR A 148	27.474	47.843	46.971	1.00	9.73	6	ATOM	1233	O	TRP A 153	44.633	41.770	52.009	1.00	7.54	8
ATOM	1181	CE2	TYR A 148	27.047	48.636	45.925	1.00	9.48	6	ATOM	1234	H	HIS A 154	44.568	39.706	52.892	1.00	7.67	7
ATOM	1182	CZ	TYR A 148	27.896	48.914	44.844	1.00	8.99	6	ATOM	1235	CA	HIS A 154	45.937	39.586	53.334	1.00	7.24	6
ATOM	1183	OH	TYR A 148	27.441	49.705	43.833	1.00	8.37	8	ATOM	1236	CB	HIS A 154	46.112	39.730	54.859	1.00	7.92	6
ATOM	1184	C	TYR A 148	29.940	46.030	50.426	1.00	10.22	6	ATOM	1237	CG	HIS A 154	45.804	41.145	55.233	1.00	8.88	6
ATOM	1185	O	TYR A 148	29.299	45.054	50.827	1.00	10.08	8	ATOM	1238	CD2	HIS A 154	44.674	41.660	55.765	1.00	9.84	6
ATOM	1186	H	SER A 149	31.224	46.159	50.757	1.00	10.07	7	ATOM	1239	ND1	HIS A 154	46.672	42.197	55.006	1.00	10.11	7
ATOM	1187	CA	SER A 149	31.879	45.141	51.584	1.00	9.72	6	ATOM	1240	CE1	HIS A 154	46.113	43.304	55.428	1.00	10.55	6
ATOM	1188	CB	SER A 149	32.256	43.886	50.787	1.00	9.55	6	ATOM	1241	NE2	HIS A 154	44.890	43.016	55.840	1.00	10.76	7
ATOM	1189	CG	SER A 149	33.396	43.185	51.181	1.00	8.96	8	ATOM	1242	C	HIS A 154	46.508	38.207	52.960	1.00	6.90	6
ATOM	1190	O	SER A 149	33.141	45.735	52.164	1.00	9.63	6	ATOM	1243	O	HIS A 154	45.778	37.294	52.603	1.00	6.75	8
ATOM	1191	O	SER A 149	33.897	46.334	51.423	1.00	9.31	8	ATOM	1244	N	TRP A 155	47.839	38.056	53.102	1.00	6.82	7
ATOM	1192	H	ASP A 150	33.270	45.588	53.502	1.00	9.75	7	ATOM	1245	CA	TRP A 155	48.508	36.802	52.800	1.00	6.92	6
ATOM	1193	CA	ASP A 150	34.497	46.155	54.053	1.00	9.98	6	ATOM	1246	CG	TRP A 155	49.994	36.800	53.254	1.00	6.54	6
ATOM	1194	CB	ASP A 150	34.153	46.816	55.365	1.00	13.89	6	ATOM	1247	CG	TRP A 155	50.190	36.808	54.726	1.00	6.55	6
ATOM	1195	CG	ASP A 150	33.646	45.849	56.403	1.00	17.64	6	ATOM	1248	CD2	TRP A 155	50.282	35.636	55.575	1.00	7.16	6
ATOM	1196	CD1	ASP A 150	33.340	44.644	56.213	1.00	18.84	8	ATOM	1249	CE2	TRP A 155	50.473	36.099	56.900	1.00	8.10	6
ATOM	1197	CD2	ASP A 150	33.560	46.260	57.579	1.00	20.98	8	ATOM	1250	CE3	TRP A 155	50.261	34.254	55.319	1.00	7.58	6
ATOM	1198	C	ASP A 150	35.545	45.049	54.125	1.00	9.95	6	ATOM	1251	CD1	TRP A 155	50.311	37.912	55.567	1.00	7.09	6
ATOM	1199	O	ASP A 150	36.570	45.334	54.761	1.00	10.38	8	ATOM	1252	NE1	TRP A 155	50.496	37.495	56.870	1.00	7.83	7
ATOM	1200	H	PIE A 151	35.472	43.865	53.541	1.00	9.49	7	ATOM	1253	CZ2	TRP A 155	50.582	35.208	57.972	1.00	9.47	6
ATOM	1201	CA	PIE A 151	36.518	42.860	53.667	1.00	8.88	6	ATOM	1254	CZ3	TRP A 155	50.372	33.377	56.355	1.00	8.70	6
ATOM	1202	CB	PIE A 151	35.932	41.523	53.167	1.00	10.40	6	ATOM	1255	CH2	TRP A 155	50.556	33.847	57.605	1.00	9.74	6
ATOM	1203	CG	PIE A 151	36.761	40.297	53.405	1.00	12.18	6	ATOM	1256	C	TRP A 155	47.807	35.600	53.420	1.00	6.90	6
ATOM	1204	CD1	PIE A 151	36.689	39.627	54.620	1.00	14.04	6	ATOM	1257	O	TRP A 155	47.749	34.576	52.755	1.00	6.82	8
ATOM	1205	CD2	PIE A 151	37.623	39.804	52.455	1.00	12.75	6	ATOM	1258	N	TYR A 156	47.293	35.659	54.655	1.00	6.91	7
ATOM	1206	CE1	PIE A 151	37.481	38.471	54.849	1.00	15.14	6	ATOM	1259	CA	TYR A 156	46.692	34.492	55.283	1.00	6.91	6
ATOM	1207	CE2	PIE A 151	38.380	38.647	52.644	1.00	12.08	6	ATOM	1260	CB	TYR A 156	46.619	34.685	56.813	1.00	7.50	6
ATOM	1208	CZ	PIE A 151	38.308	37.976	53.849	1.00	13.39	6	ATOM	1261	CG	TYR A 156	46.056	36.003	57.270	1.00	8.16	6
ATOM	1209	C	PIE A 151	37.748	43.217	52.864	1.00	8.54	6	ATOM	1262	CD1	TYR A 156	44.665	36.114	57.420	1.00	8.64	6
ATOM	1210	O	PIE A 151	37.762	43.556	51.675	1.00	8.21	8	ATOM	1263	CE1	TYR A 156	44.049	37.302	57.839	1.00	8.68	6
ATOM	1211	H	LYS A 152	38.899	43.119	53.477	1.00	8.50	7	ATOM	1264	CD2	TYR A 156	46.829	37.094	57.597	1.00	8.54	6
ATOM	1212	CA	LYS A 152	40.228	43.377	52.979	1.00	8.62	6	ATOM	1265	CE2	TYR A 156	46.254	38.298	58.052	1.00	8.83	6
ATOM	1213	CB	LYS A 152	40.989	44.385	53.849	1.00	10.86	6	ATOM	1266	CZ	TYR A 156	44.870	38.365	58.159	1.00	8.97	6
ATOM	1214	CG	LYS A 152	40.384	45.787	54.073	1.00	11.07	6	ATOM	1267	OH	TYR A 156	44.271	39.510	58.597	1.00	9.48	8
ATOM	1215	CD	LYS A 152	39.941	46.481	52.798	1.00	11.11	6	ATOM	1268	C	TYR A 156	45.351	34.041	54.691	1.00	6.48	8
ATOM	1216	CE	LYS A 152	39.350	47.830	53.236	1.00	12.45	6	ATOM	1269	O	TYR A 156	44.907	32.991	55.146	1.00	6.37	8
ATOM	1217	HZ	LYS A 152	38.434	48.440	52.290	1.00	15.39	7	ATOM	1270	N	HIS A 157	44.751	34.691	53.719	1.00	5.96	7
ATOM	1218	C	LYS A 152	41.038	42.082	52.958	1.00	8.53	6	ATOM	1271	CA	HIS A 157	43.567	34.321	53.016	1.00	5.71	6
ATOM	1219	O	LYS A 152	40.938	41.290	53.892	1.00	8.53	8	ATOM	1272	CB	HIS A 157	42.768	35.566	52.552	1.00	5.00	6

ATOM	1273	CG	HIS A 157	42.236	36.398	53.732	1.00	5.00	6	ATOM	1326	C23	TRP A 163	59.639	37.017	39.046	1.00	14.61	6
ATOM	1274	CD2	HIS A 157	41.620	36.018	54.866	1.00	5.00	6	ATOM	1327	CH2	TRP A 163	60.210	38.279	39.139	1.00	16.01	6
ATOM	1275	H01	HIS A 157	42.426	37.765	53.793	1.00	5.10	7	ATOM	1328	C	TRP A 163	57.008	35.969	44.102	1.00	12.82	6
ATOM	1276	CE1	HIS A 157	41.880	38.216	54.935	1.00	6.49	6	ATOM	1329	O	TRP A 163	56.225	36.180	45.012	1.00	12.72	8
ATOM	1277	HE2	HIS A 157	41.398	37.147	55.588	1.00	5.12	7	ATOM	1330	N	TRP A 164	58.298	36.130	44.243	1.00	13.51	7
ATOM	1278	C	HIS A 157	43.896	33.473	51.753	1.00	5.75	6	ATOM	1331	CA	ASP A 164	58.961	36.679	45.420	1.00	14.00	6
ATOM	1279	O	HIS A 157	43.028	33.056	50.978	1.00	5.63	8	ATOM	1332	CB	ASP A 164	60.073	35.796	45.937	1.00	13.67	6
ATOM	1280	H	PIE A 158	45.182	33.311	51.471	1.00	5.60	7	ATOM	1333	CG	ASP A 164	60.891	36.513	47.003	1.00	14.44	6
ATOM	1281	CA	PIE A 158	45.722	32.597	50.312	1.00	5.84	6	ATOM	1334	CO1	ASP A 164	60.392	37.464	47.682	1.00	14.14	8
ATOM	1282	CB	PIE A 158	46.578	33.527	49.412	1.00	5.00	6	ATOM	1335	CO2	ASP A 164	62.070	36.096	47.155	1.00	15.41	8
ATOM	1283	CG	PIE A 158	45.867	34.784	48.992	1.00	5.00	6	ATOM	1336	C	ASP A 164	59.560	38.004	44.913	1.00	14.37	6
ATOM	1284	CD1	PIE A 158	46.099	35.994	49.658	1.00	5.00	6	ATOM	1337	O	ASP A 164	60.491	37.969	44.125	1.00	14.14	8
ATOM	1285	CD2	PIE A 158	44.972	34.788	47.942	1.00	5.00	6	ATOM	1338	N	GLU A 165	59.024	39.109	45.390	1.00	14.96	7
ATOM	1286	CE1	PIE A 158	45.418	37.147	49.286	1.00	6.00	6	ATOM	1339	CA	GLU A 165	59.449	40.429	44.953	1.00	15.64	6
ATOM	1287	CE2	PIE A 158	44.300	35.931	47.568	1.00	5.36	6	ATOM	1340	CB	GLU A 165	58.453	41.456	45.446	1.00	15.08	6
ATOM	1288	CZ	PIE A 158	44.494	37.129	48.230	1.00	5.65	6	ATOM	1341	CG	GLU A 165	58.724	42.887	45.070	1.00	16.95	6
ATOM	1289	C	PIE A 158	46.580	31.365	50.692	1.00	5.86	6	ATOM	1342	CD	GLU A 165	58.627	43.079	43.584	1.00	18.88	6
ATOM	1290	O	PIE A 158	47.192	31.311	51.800	1.00	5.98	8	ATOM	1343	OE1	GLU A 165	59.126	44.095	43.075	1.00	22.59	8
ATOM	1291	N	ASP A 159	46.638	30.354	49.804	1.00	5.59	7	ATOM	1344	OE2	GLU A 165	58.071	42.288	42.822	1.00	19.30	8
ATOM	1292	CA	ASP A 159	47.461	29.211	50.022	1.00	5.30	6	ATOM	1345	C	GLU A 165	60.843	40.736	45.498	1.00	16.33	6
ATOM	1293	CB	ASP A 159	46.924	27.979	49.262	1.00	5.00	6	ATOM	1346	O	GLU A 165	61.504	41.590	44.951	1.00	16.30	8
ATOM	1294	CG	ASP A 159	45.876	27.378	50.090	1.00	5.58	6	ATOM	1347	N	SER A 166	61.227	40.104	46.593	1.00	16.71	7
ATOM	1295	CO1	ASP A 159	45.988	27.501	51.360	1.00	8.12	8	ATOM	1348	CA	SER A 166	62.499	40.241	47.255	1.00	17.23	6
ATOM	1296	CO2	ASP A 159	44.852	26.813	49.700	1.00	5.00	8	ATOM	1349	CB	SER A 166	62.471	39.215	48.415	1.00	17.88	6
ATOM	1297	C	ASP A 159	48.878	29.377	49.478	1.00	5.70	6	ATOM	1350	CG	SER A 166	63.157	39.838	49.443	1.00	21.31	8
ATOM	1298	O	ASP A 159	49.808	28.719	49.999	1.00	6.04	8	ATOM	1351	C	SER A 166	63.694	39.857	46.363	1.00	17.59	6
ATOM	1299	N	GLY A 160	49.083	30.164	48.444	1.00	5.67	7	ATOM	1352	O	SER A 166	64.511	40.670	45.931	1.00	17.48	8
ATOM	1300	CA	GLY A 160	50.438	30.251	47.914	1.00	6.24	6	ATOM	1353	N	ARG A 167	63.756	38.534	46.062	1.00	17.53	7
ATOM	1301	C	GLY A 160	50.472	31.296	46.798	1.00	6.82	6	ATOM	1354	CA	ARG A 167	64.754	37.962	45.202	1.00	17.50	6
ATOM	1302	O	GLY A 160	49.389	31.807	46.477	1.00	6.74	8	ATOM	1355	CB	ARG A 167	64.972	36.483	45.538	1.00	18.49	6
ATOM	1303	N	ALA A 161	51.622	31.520	46.224	1.00	7.20	7	ATOM	1356	CG	ARG A 167	65.372	36.319	46.984	1.00	19.67	6
ATOM	1304	CA	ALA A 161	51.756	32.488	45.174	1.00	8.08	6	ATOM	1357	CD	ARG A 167	65.413	34.810	47.294	1.00	22.11	6
ATOM	1305	CB	ALA A 161	52.023	33.869	45.775	1.00	8.88	6	ATOM	1358	NE	ARG A 167	65.554	34.699	48.736	1.00	24.69	7
ATOM	1306	C	ALA A 161	52.933	32.083	44.297	1.00	9.05	6	ATOM	1359	CZ	ARG A 167	64.638	35.047	49.658	1.00	27.34	6
ATOM	1307	O	ALA A 161	53.582	31.055	44.591	1.00	8.86	8	ATOM	1360	HI1	ARG A 167	63.420	35.550	49.443	1.00	24.66	7
ATOM	1308	N	ASP A 162	53.158	32.846	43.215	1.00	10.00	7	ATOM	1361	HI2	ARG A 167	65.027	34.853	50.954	1.00	28.95	7
ATOM	1309	CA	ASP A 162	54.278	32.418	42.372	1.00	11.36	6	ATOM	1362	C	ARG A 167	64.344	38.047	43.729	1.00	17.36	6
ATOM	1310	CB	ASP A 162	53.786	32.031	40.983	1.00	15.10	6	ATOM	1363	O	ARG A 167	65.179	37.757	42.880	1.00	17.29	8
ATOM	1311	CG	ASP A 162	53.111	33.242	40.352	1.00	19.35	6	ATOM	1364	N	LYS A 168	63.124	38.406	43.386	1.00	17.25	7
ATOM	1312	CO1	ASP A 162	52.930	34.331	40.947	1.00	19.47	8	ATOM	1365	CA	LYS A 168	62.636	38.491	42.048	1.00	17.27	6
ATOM	1313	CO2	ASP A 162	52.725	32.956	39.169	1.00	22.93	8	ATOM	1366	CB	LYS A 168	63.318	39.579	41.203	1.00	20.36	6
ATOM	1314	C	ASP A 162	55.381	33.455	42.149	1.00	11.95	6	ATOM	1367	CG	LYS A 168	62.818	40.920	41.752	1.00	23.95	6
ATOM	1315	O	ASP A 162	56.107	33.336	41.131	1.00	12.10	8	ATOM	1368	CD	LYS A 168	63.605	42.120	41.269	1.00	26.67	6
ATOM	1316	N	TRP A 163	55.489	34.435	43.048	1.00	12.03	7	ATOM	1369	CE	LYS A 168	62.855	43.415	41.686	1.00	28.90	6
ATOM	1317	CA	TRP A 163	56.533	35.418	42.793	1.00	12.34	6	ATOM	1370	HZ	LYS A 168	62.830	43.494	43.201	1.00	30.66	7
ATOM	1318	CB	TRP A 163	55.954	36.485	41.881	1.00	13.20	6	ATOM	1371	C	LYS A 168	62.766	37.148	41.332	1.00	17.23	6
ATOM	1319	CG	TRP A 163	56.925	37.600	41.631	1.00	13.20	6	ATOM	1372	O	LYS A 168	63.337	37.062	40.229	1.00	17.13	8
ATOM	1320	CD2	TRP A 163	58.014	37.602	40.715	1.00	14.18	6	ATOM	1373	N	LYS A 169	62.203	36.106	41.956	1.00	16.95	7
ATOM	1321	CE1	TRP A 163	58.646	38.869	40.826	1.00	15.32	6	ATOM	1374	CA	LYS A 169	62.199	34.766	41.380	1.00	16.59	6
ATOM	1322	CE2	TRP A 163	58.520	36.667	39.803	1.00	14.71	6	ATOM	1375	CB	LYS A 169	63.086	33.751	42.115	1.00	17.17	6
ATOM	1323	CD1	TRP A 163	58.950	38.813	42.245	1.00	13.62	6	ATOM	1376	CG2	LYS A 169	64.599	34.139	42.040	1.00	16.91	6
ATOM	1324	HE1	TRP A 163	57.980	39.589	41.774	1.00	13.74	7	ATOM	1377	CG1	LYS A 169	62.641	33.597	43.557	1.00	17.77	6
ATOM	1325	CZ2	TRP A 163	59.757	39.243	40.036	1.00	16.07	6	ATOM	1378	CD1	LYS A 169	63.595	32.811	44.434	1.00	18.17	6

1379	ATOH	C	ILE A 169	60.748	34.265	41.354	1.00	16.43	6	1432	ATOH	CE1	PIIE A 175	50.443	33.823	50.320	1.00	7.64	6
1380	ATOH	O	ILE A 169	59.894	34.602	42.175	1.00	15.97	8	1433	ATOH	CE2	PIIE A 175	52.585	33.103	49.614	1.00	6.81	6
1381	ATOH	N	SER A 170	60.458	33.469	40.342	1.00	16.39	7	1434	ATOH	CZ	PIIE A 175	51.517	33.983	49.476	1.00	7.21	6
1382	ATOH	CA	SER A 170	59.209	32.808	40.120	1.00	16.32	6	1435	ATOH	C	PIIE A 175	52.567	28.942	53.770	1.00	11.49	6
1383	ATOH	CB	SER A 170	58.830	32.767	38.642	1.00	18.20	6	1436	ATOH	O	PIIE A 175	51.868	27.912	53.875	1.00	11.44	8
1384	ATOH	OG	SER A 170	57.519	32.181	38.607	1.00	22.81	8	1437	ATOH	N	PIIE A 175	53.288	29.352	54.813	1.00	11.77	7
1385	ATOH	C	SER A 170	59.306	31.335	40.518	1.00	16.18	6	1438	ATOH	CA	ARG A 176	53.328	28.725	56.129	1.00	12.20	6
1386	ATOH	O	SER A 170	60.106	30.599	39.908	1.00	16.17	8	1439	ATOH	CB	ARG A 176	54.684	28.802	56.775	1.00	13.53	6
1387	ATOH	N	ARG A 171	58.531	30.882	41.508	1.00	15.84	7	1440	ATOH	CG	ARG A 176	55.768	27.776	56.372	1.00	14.88	6
1388	ATOH	CA	ARG A 171	58.504	29.492	41.954	1.00	15.28	6	1441	ATOH	CO	ARG A 176	55.188	26.438	56.823	1.00	15.37	6
1389	ATOH	CG	ARG A 171	59.448	29.168	43.104	1.00	17.32	6	1442	ATOH	NE	ARG A 176	56.133	25.355	56.737	1.00	15.69	7
1390	ATOH	CG	ARG A 171	60.894	29.497	43.152	1.00	19.88	6	1443	ATOH	CZ	ARG A 176	56.118	24.277	55.962	1.00	16.02	6
1391	ATOH	CD	ARG A 171	61.825	28.448	42.555	1.00	23.48	6	1444	ATOH	NH1	ARG A 176	55.150	24.037	55.065	1.00	16.35	7
1392	ATOH	NE	ARG A 171	63.204	28.981	42.466	1.00	27.05	7	1445	ATOH	NH2	ARG A 176	57.151	23.430	56.062	1.00	16.02	7
1393	ATOH	CZ	ARG A 171	63.661	29.577	41.358	1.00	29.43	6	1446	ATOH	C	ARG A 176	52.330	29.526	56.994	1.00	12.82	6
1394	ATOH	NH1	ARG A 171	62.909	29.718	40.256	1.00	30.87	7	1447	ATOH	O	ARG A 176	52.303	30.774	56.778	1.00	12.92	8
1395	ATOH	NH2	ARG A 171	64.884	30.070	41.191	1.00	30.59	7	1448	ATOH	N	GLY A 177	51.560	28.911	57.850	1.00	13.07	7
1396	ATOH	C	ARG A 171	57.052	29.164	42.380	1.00	14.63	6	1449	ATOH	CA	GLY A 177	50.590	29.656	58.637	1.00	13.84	6
1397	ATOH	O	ARG A 171	56.203	30.055	42.313	1.00	14.71	8	1450	ATOH	C	GLY A 177	49.736	28.715	59.449	1.00	14.51	6
1398	ATOH	N	ILE A 172	56.737	27.949	42.824	1.00	13.80	7	1451	ATOH	O	GLY A 177	50.056	27.482	59.489	1.00	15.11	8
1399	ATOH	CA	ILE A 172	55.389	27.671	43.336	1.00	13.02	6	1452	ATOH	N	GLU A 178	48.649	29.125	60.069	1.00	14.47	7
1400	ATOH	CB	ILE A 172	54.752	26.357	42.862	1.00	11.93	6	1453	ATOH	CA	GLU A 178	47.810	28.222	60.859	1.00	14.86	6
1401	ATOH	CG1	ILE A 172	53.502	26.058	43.656	1.00	11.06	6	1454	ATOH	CG	GLU A 178	46.912	29.021	61.833	1.00	15.74	6
1402	ATOH	CG1	ILE A 172	54.360	26.386	41.354	1.00	11.59	6	1455	ATOH	CG	GLU A 178	47.575	29.715	63.000	1.00	16.47	6
1403	ATOH	CG1	ILE A 172	53.920	25.010	40.927	1.00	12.67	6	1456	ATOH	CD	GLU A 178	48.458	28.762	63.819	1.00	18.26	6
1404	ATOH	C	ILE A 172	55.639	27.730	44.867	1.00	12.55	6	1457	ATOH	OE1	GLU A 178	48.216	27.504	63.969	1.00	19.50	8
1405	ATOH	O	ILE A 172	56.218	26.808	45.469	1.00	12.52	8	1458	ATOH	OE2	GLU A 178	49.488	29.266	64.326	1.00	16.85	8
1406	ATOH	N	PIIE A 173	55.290	28.812	45.529	1.00	11.95	7	1459	ATOH	C	GLU A 178	46.961	27.310	59.957	1.00	15.02	6
1407	ATOH	CA	PIIE A 173	55.464	28.982	46.956	1.00	11.52	6	1460	ATOH	O	GLU A 178	46.138	27.801	59.151	1.00	15.35	8
1408	ATOH	CB	PIIE A 173	55.813	30.424	47.326	1.00	8.63	6	1461	ATOH	N	GLY A 179	47.148	26.015	60.032	1.00	14.81	7
1409	ATOH	CG	PIIE A 173	57.088	30.932	46.719	1.00	8.19	6	1462	ATOH	CA	GLY A 179	46.450	25.042	59.221	1.00	14.68	6
1410	ATOH	CD1	PIIE A 173	57.085	31.845	45.697	1.00	6.97	6	1463	ATOH	C	GLY A 179	46.692	25.221	57.702	1.00	14.28	6
1411	ATOH	CD2	PIIE A 173	58.313	30.470	47.211	1.00	8.07	6	1464	ATOH	O	GLY A 179	45.709	24.906	56.979	1.00	14.54	8
1412	ATOH	CE1	PIIE A 173	58.277	32.307	45.123	1.00	8.07	6	1465	ATOH	N	LYS A 180	47.854	25.708	57.243	1.00	13.43	7
1413	ATOH	CE2	PIIE A 173	59.512	30.949	46.686	1.00	8.69	6	1466	ATOH	CA	LYS A 180	48.022	25.959	55.824	1.00	12.55	6
1414	ATOH	CZ	PIIE A 173	59.484	31.844	45.607	1.00	7.75	6	1467	ATOH	CB	LYS A 180	49.163	26.955	55.631	1.00	11.48	6
1415	ATOH	C	PIIE A 173	53.109	29.085	47.372	1.00	11.50	6	1468	ATOH	CG	LYS A 180	48.825	28.409	55.816	1.00	11.89	6
1416	ATOH	O	PIIE A 173	54.257	27.696	48.657	1.00	11.79	8	1469	ATOH	CD	LYS A 180	47.710	28.914	54.938	1.00	9.28	6
1417	ATOH	N	LYS A 174	53.185	27.303	49.524	1.00	11.02	6	1470	ATOH	CE	LYS A 180	47.355	30.371	55.116	1.00	9.37	6
1418	ATOH	CA	LYS A 174	52.045	25.443	50.770	1.00	6.03	6	1471	ATOH	NZ	LYS A 180	46.097	30.683	54.339	1.00	9.60	7
1419	ATOH	CB	LYS A 174	53.268	25.849	49.981	1.00	7.54	6	1472	ATOH	C	LYS A 180	48.271	24.676	55.037	1.00	12.15	6
1420	ATOH	CG	LYS A 174	52.045	25.443	50.770	1.00	6.03	6	1473	ATOH	O	LYS A 180	49.150	23.919	55.465	1.00	12.30	8
1421	ATOH	CD	LYS A 174	51.800	23.947	50.993	1.00	5.90	6	1474	ATOH	N	ALA A 181	47.571	24.402	53.925	1.00	11.19	7
1422	ATOH	CE	LYS A 174	53.109	23.439	51.713	1.00	6.00	6	1475	ATOH	CA	ALA A 181	47.792	23.208	53.139	1.00	10.23	6
1423	ATOH	NZ	LYS A 174	52.991	22.034	52.176	1.00	5.20	7	1476	ATOH	CB	ALA A 181	47.183	21.975	53.825	1.00	8.27	6
1424	ATOH	C	LYS A 174	53.313	28.195	50.787	1.00	11.19	6	1477	ATOH	C	ALA A 181	47.120	23.287	51.761	1.00	9.57	6
1425	ATOH	O	LYS A 174	54.402	28.117	51.406	1.00	11.32	8	1478	ATOH	O	ALA A 181	46.125	23.952	51.862	1.00	8.95	8
1426	ATOH	N	PIIE A 175	52.357	28.950	51.264	1.00	11.10	7	1479	ATOH	N	TRP A 182	47.457	22.762	50.604	1.00	8.86	7
1427	ATOH	CA	PIIE A 175	52.555	29.759	52.486	1.00	11.23	6	1480	ATOH	CA	TRP A 182	46.604	22.929	49.465	1.00	8.54	6
1428	ATOH	CB	PIIE A 175	51.440	30.845	52.516	1.00	9.58	6	1481	ATOH	CG	TRP A 182	47.232	22.145	48.309	1.00	6.73	6
1429	ATOH	CG	PIIE A 175	51.497	31.920	51.427	1.00	9.11	6	1482	ATOH	CG	TRP A 182	48.624	22.609	47.966	1.00	5.79	6
1430	ATOH	CD1	PIIE A 175	50.410	32.806	51.283	1.00	8.73	6	1483	ATOH	CD2	TRP A 182	49.003	23.922	47.558	1.00	5.00	6
1431	ATOH	CD2	PIIE A 175	52.569	32.097	50.557	1.00	7.13	6	1484	ATOH	CE2	TRP A 182	50.388	23.887	47.314	1.00	5.13	6

1485	CE3	TRP	A	182	48.278	25.127	47.361	1.00	5.00	6	ATOH
1486	CD1	TRP	A	182	49.768	21.861	48.002	1.00	5.63	6	ATOH
1487	HE1	TRP	A	182	50.860	22.616	47.616	1.00	5.04	7	ATOH
1488	CZ2	TRP	A	182	51.110	25.022	46.895	1.00	5.00	6	ATOH
1489	CZ3	TRP	A	182	48.966	26.236	46.927	1.00	5.00	6	ATOH
1490	CI2	TRP	A	182	50.376	26.186	46.723	1.00	5.00	6	ATOH
1491	C	TRP	A	182	45.218	22.348	49.787	1.00	8.52	6	ATOH
1492	O	TRP	A	182	45.029	21.400	50.552	1.00	8.24	8	ATOH
1493	H	ASP	A	183	44.187	22.939	49.183	1.00	8.61	7	ATOH
1494	CA	ASP	A	183	42.814	22.546	49.339	1.00	8.57	6	ATOH
1495	CB	ASP	A	183	41.746	23.407	48.669	1.00	7.64	6	ATOH
1496	CG	ASP	A	183	41.829	24.846	49.207	1.00	7.97	6	ATOH
1497	OD1	ASP	A	183	42.136	25.011	50.384	1.00	5.19	8	ATOH
1498	OD2	ASP	A	183	41.604	25.903	48.623	1.00	7.20	8	ATOH
1499	C	ASP	A	183	42.678	21.163	48.661	1.00	8.68	6	ATOH
1500	O	ASP	A	183	43.392	20.764	47.757	1.00	8.29	8	ATOH
1501	H	TRP	A	184	41.655	20.526	49.221	1.00	8.85	7	ATOH
1502	CA	TRP	A	184	41.337	19.214	48.816	1.00	9.31	6	ATOH
1503	CB	TRP	A	184	42.068	18.015	49.485	1.00	9.16	6	ATOH
1504	CG	TRP	A	184	41.858	16.719	48.814	1.00	9.24	6	ATOH
1505	CD2	TRP	A	184	42.391	16.211	47.580	1.00	9.64	6	ATOH
1506	CE2	TRP	A	184	41.870	14.896	47.384	1.00	9.60	6	ATOH
1507	CE3	TRP	A	184	43.240	16.730	46.594	1.00	8.61	6	ATOH
1508	CD1	TRP	A	184	41.009	15.713	49.300	1.00	10.78	6	ATOH
1509	HE1	TRP	A	184	41.019	14.620	48.426	1.00	9.86	7	ATOH
1510	CZ2	TRP	A	184	42.149	14.151	46.250	1.00	9.85	6	ATOH
1511	CZ3	TRP	A	184	43.547	15.968	45.479	1.00	9.71	6	ATOH
1512	CH2	TRP	A	184	43.008	14.693	45.314	1.00	9.96	6	ATOH
1513	C	TRP	A	184	39.766	18.960	48.936	1.00	9.76	6	ATOH
1514	O	TRP	A	184	39.093	19.322	49.789	1.00	10.01	8	ATOH
1515	H	GLU	A	185	39.594	18.432	47.785	1.00	9.88	7	ATOH
1516	CA	GLU	A	185	39.263	17.724	46.655	1.00	9.32	6	ATOH
1517	CB	GLU	A	185	38.201	16.707	46.321	1.00	11.41	6	ATOH
1518	CG	GLU	A	185	38.829	15.901	45.132	1.00	13.77	6	ATOH
1519	CD	GLU	A	185	38.070	14.631	44.814	1.00	14.04	8	ATOH
1520	OE1	GLU	A	185	37.147	14.228	45.559	1.00	14.41	8	ATOH
1521	OE2	GLU	A	185	38.349	14.001	43.768	1.00	14.04	8	ATOH
1522	C	GLU	A	185	39.394	18.759	45.479	1.00	8.78	6	ATOH
1523	O	GLU	A	185	38.591	19.636	45.294	1.00	8.92	8	ATOH
1524	H	VAL	A	186	40.502	18.566	44.792	1.00	8.34	7	ATOH
1525	CA	VAL	A	186	40.810	19.326	43.583	1.00	8.33	6	ATOH
1526	CB	VAL	A	186	41.807	20.506	43.583	1.00	8.32	6	ATOH
1527	CG1	VAL	A	186	41.196	21.617	44.616	1.00	7.05	6	ATOH
1528	CG2	VAL	A	186	43.173	20.110	44.308	1.00	5.20	6	ATOH
1529	C	VAL	A	186	41.364	18.291	42.578	1.00	8.42	6	ATOH
1530	O	VAL	A	186	41.505	17.111	42.956	1.00	8.25	8	ATOH
1531	H	SER	A	187	41.735	18.666	41.367	1.00	8.40	7	ATOH
1532	CA	SER	A	187	42.313	17.723	40.445	1.00	8.96	6	ATOH
1533	CB	SER	A	187	42.664	18.422	39.113	1.00	8.95	6	ATOH
1534	CG	SER	A	187	43.472	17.537	38.328	1.00	8.65	8	ATOH
1535	C	SER	A	187	43.603	17.153	41.060	1.00	9.46	6	ATOH
1536	O	SER	A	187	44.375	17.887	41.684	1.00	9.28	8	ATOH
1537	H	SER	A	188	43.908	15.846	40.823	1.00	9.77	7	ATOH

1591	ATOH	1591	O	ASP A 194	45.143	25.681	42.616	1.00	6.42	8
1592	ATOH	1592	N	YR A 195	47.129	24.919	43.145	1.00	6.43	7
1593	ATOH	1593	CA	YR A 195	47.781	26.059	42.596	1.00	6.19	6
1594	ATOH	1594	CB	YR A 195	49.261	26.101	43.153	1.00	5.52	6
1595	ATOH	1595	CG	YR A 195	49.722	27.472	42.821	1.00	5.15	6
1596	ATOH	1596	CD	YR A 195	49.314	28.569	43.582	1.00	5.28	6
1597	ATOH	1597	CE	YR A 195	49.676	29.862	43.186	1.00	5.27	6
1598	ATOH	1598	CE	YR A 195	50.456	27.686	41.665	1.00	5.05	6
1599	ATOH	1599	CE	YR A 195	50.809	28.972	41.246	1.00	5.06	6
1600	ATOH	1600	CZ	YR A 195	50.386	30.053	42.030	1.00	5.27	6
1601	ATOH	1601	OH	YR A 195	50.742	31.310	41.636	1.00	5.27	8
1602	ATOH	1602	C	YR A 195	48.128	25.186	40.392	1.00	6.73	6
1603	ATOH	1603	O	YR A 196	47.329	27.323	40.580	1.00	7.17	7
1604	ATOH	1604	N	LEU A 196	45.962	27.721	38.510	1.00	6.89	6
1605	ATOH	1605	CA	LEU A 196	44.578	28.516	36.621	1.00	7.71	6
1606	ATOH	1606	CB	LEU A 196	46.520	26.975	36.126	1.00	6.67	6
1607	ATOH	1607	CG	LEU A 196	48.181	28.816	38.807	1.00	7.86	6
1608	ATOH	1608	CD	LEU A 196	49.162	28.671	38.073	1.00	7.98	8
1609	ATOH	1609	C	LEU A 196	47.861	29.990	39.319	1.00	7.94	7
1610	ATOH	1610	N	HET A 197	48.577	31.228	39.029	1.00	8.00	6
1611	ATOH	1611	CA	HET A 197	48.230	31.699	37.645	1.00	11.16	6
1612	ATOH	1612	CB	HET A 197	46.758	32.064	37.445	1.00	15.62	6
1613	ATOH	1613	CG	HET A 197	46.223	32.419	35.732	1.00	22.83	16
1614	ATOH	1614	CD	HET A 197	47.695	33.237	35.117	1.00	21.60	6
1615	ATOH	1615	CE	HET A 197	48.157	32.310	40.032	1.00	7.71	6
1616	ATOH	1616	C	HET A 197	47.200	32.162	40.792	1.00	7.22	8
1617	ATOH	1617	O	HET A 197	48.875	33.421	39.997	1.00	7.95	7
1618	ATOH	1618	N	YR A 198	48.725	34.595	40.849	1.00	8.22	6
1619	ATOH	1619	CA	YR A 198	47.512	35.420	40.476	1.00	9.23	6
1620	ATOH	1620	CB	YR A 198	47.601	35.991	39.081	1.00	10.99	6
1621	ATOH	1621	CG	YR A 198	46.600	35.690	38.145	1.00	11.90	6
1622	ATOH	1622	CD	YR A 198	46.655	36.230	36.875	1.00	12.83	6
1623	ATOH	1623	C	YR A 198	48.664	36.817	38.741	1.00	11.91	6
1624	ATOH	1624	N	YR A 198	48.745	37.364	37.443	1.00	12.82	6
1625	ATOH	1625	CA	YR A 198	47.741	37.045	36.538	1.00	13.43	6
1626	ATOH	1626	CB	YR A 198	47.797	37.589	35.261	1.00	14.37	8
1627	ATOH	1627	CG	YR A 198	48.629	34.167	42.312	1.00	7.86	6
1628	ATOH	1628	CD	YR A 198	49.362	33.257	42.693	1.00	7.88	8
1629	ATOH	1629	C	YR A 198	47.769	34.787	43.117	1.00	7.31	7
1630	ATOH	1630	N	YR A 199	47.563	34.481	44.537	1.00	6.22	6
1631	ATOH	1631	CA	YR A 199	47.321	35.767	45.359	1.00	6.68	6
1632	ATOH	1632	CB	YR A 199	45.255	33.918	44.687	1.00	5.38	6
1633	ATOH	1633	CG	YR A 199	46.702	32.319	45.148	1.00	5.09	7
1634	ATOH	1634	CD	YR A 199	45.748	31.224	45.295	1.00	5.00	6
1635	ATOH	1635	C	YR A 199	46.567	29.901	45.278	1.00	5.25	6
1636	ATOH	1636	N	YR A 200	45.495	28.798	45.141	1.00	6.80	6
1637	ATOH	1637	CA	YR A 200	44.912	28.830	44.024	1.00	6.41	8
1638	ATOH	1638	CB	YR A 200	45.139	27.965	46.011	1.00	6.48	8
1639	ATOH	1639	CG	YR A 200	44.879	31.313	46.526	1.00	5.00	6
1640	ATOH	1640	CD	YR A 200						
1641	ATOH	1641	C	YR A 200						
1642	ATOH	1642	N	YR A 200						
1643	ATOH	1643	CA	YR A 200						
1644	ATOH	1644	CB	YR A 200						
1645	ATOH	1645	CG	YR A 200						
1646	ATOH	1646	CD	YR A 200						
1647	ATOH	1647	C	YR A 200						
1648	ATOH	1648	N	YR A 200						
1649	ATOH	1649	CA	YR A 200						
1650	ATOH	1650	CB	YR A 200						
1651	ATOH	1651	CG	YR A 200						
1652	ATOH	1652	CD	YR A 200						
1653	ATOH	1653	C	YR A 200						
1654	ATOH	1654	N	YR A 200						
1655	ATOH	1655	CA	YR A 200						
1656	ATOH	1656	CB	YR A 200						
1657	ATOH	1657	CG	YR A 200						
1658	ATOH	1658	CD	YR A 200						
1659	ATOH	1659	C	YR A 200						
1660	ATOH	1660	N	YR A 200						
1661	ATOH	1661	CA	YR A 200						
1662	ATOH	1662	CB	YR A 200						
1663	ATOH	1663	CG	YR A 200						
1664	ATOH	1664	CD	YR A 200						
1665	ATOH	1665	C	YR A 200						
1666	ATOH	1666	N	YR A 200						
1667	ATOH	1667	CA	YR A 200						
1668	ATOH	1668	CB	YR A 200						
1669	ATOH	1669	CG	YR A 200						
1670	ATOH	1670	CD	YR A 200						
1671	ATOH	1671	C	YR A 200						
1672	ATOH	1672	N	YR A 200						
1673	ATOH	1673	CA	YR A 200						
1674	ATOH	1674	CB	YR A 200						
1675	ATOH	1675	CG	YR A 200						
1676	ATOH	1676	CD	YR A 200						
1677	ATOH	1677	C	YR A 200						
1678	ATOH	1678	N	YR A 200						
1679	ATOH	1679	CA	YR A 200						
1680	ATOH	1680	CB	YR A 200						
1681	ATOH	1681	CG	YR A 200						
1682	ATOH	1682	CD	YR A 200						
1683	ATOH	1683	C	YR A 200						
1684	ATOH	1684	N	YR A 200						
1685	ATOH	1685	CA	YR A 200						
1686	ATOH	1686	CB	YR A 200						
1687	ATOH	1687	CG	YR A 200						
1688	ATOH	1688	CD	YR A 200						
1689	ATOH	1689	C	YR A 200						
1690	ATOH	1690	N	YR A 200						
1691	ATOH	1691	CA	YR A 200						
1692	ATOH	1692	CB	YR A 200						
1693	ATOH	1693	CG	YR A 200						
1694	ATOH	1694	CD	YR A 200						
1695	ATOH	1695	C	YR A 200						
1696	ATOH	1696	N	YR A 200						

1697	1698	1699	1700	1701	1702	1703	1704	1705	1706	1707	1708	1709	1710	1711	1712	1713	1714	1715	1716	1717	1718	1719	1720	1721	1722	1723	1724	1725	1726	1727	1728	1729	1730	1731	1732	1733	1734	1735	1736	1737	1738	1739	1740	1741	1742	1743	1744	1745	1746	1747	1748	1749	
ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	ATOH	
H	CA	CB	CG	CD	CE	CF	CG	CH	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR	CS	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG	DH	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU	DV	DW	DX	DY	DZ	
ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207	ASP A 207		
36.466	36.056	36.934	36.964	36.208	37.779	36.033	35.225	36.985	37.054	38.353	38.292	39.526	35.795	35.103	35.436	34.257	34.140	32.865	32.996	32.199	32.798	31.623	31.558	31.490	30.401	32.614	32.662	34.061	34.267	33.197	32.845	32.747	32.384	31.758	32.907	32.727	33.705	35.056	33.560	33.276	30.724	30.604	29.168	28.634	29.076	29.312	28.914	28.352	27.462	28.687			
32.591	33.949	35.059	35.075	34.392	35.836	34.139	34.906	33.441	33.472	32.859	32.594	33.788	32.784	33.349	31.598	30.881	29.527	28.638	28.784	31.743	31.882	33.165	33.591	34.416	34.806	35.095	36.296	36.946	38.168	39.270	39.772	36.053	36.890	34.572	33.464	33.934	33.139	34.155	34.456	33.516	33.214	32.331	30.863	30.065	28.701	27.848	34.524	34.755	35.476				
56.971	56.613	57.168	58.705	59.396	59.261	55.096	54.573	54.427	52.973	52.465	50.949	52.805	52.426	51.530	52.923	52.457	53.170	52.878	52.814	52.652	51.884	54.102	55.584	53.261	52.803	53.060	52.216	52.363	51.517	51.640	50.515	52.771	50.721	50.060	48.781	48.413	46.939	48.636	47.522	49.424	50.553	50.321	51.592	51.442	52.609	49.417	48.620	50.279					
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
6.12	6.05	6.37	6.87	6.00	7.95	6.17	5.78	6.47	6.58	7.47	7.06	6.71	6.90	6.95	6.93	7.00	5.34	5.00	5.00	7.32	7.35	7.52	7.62	7.58	7.48	7.67	7.90	9.96	13.89	16.28	18.47	13.34	7.61	7.56	7.17	8.17	9.40	7.69	6.87	6.92	7.14	6.97	9.86	10.33	11.44	7.15	6.94	7.01					
28.061	28.638	28.423	29.354	29.770	31.138	28.290	27.317	29.481	29.726	31.216	31.353	31.418	31.427	31.455	31.355	31.418	31.507	31.494	31.534	28.836	28.222	27.936	26.482	25.868	25.955	24.531	24.011	22.627	23.923	24.065	23.541	25.329	26.556	26.778	27.638	27.466	28.514	26.112	26.535	28.169	29.215	29.058	25.395	24.708	26.300	26.537	27.703	28.243	28.615				
36.774	37.530	39.011	39.548	41.017	41.472	37.533	38.174	37.502	38.173	38.139	38.622	37.741	38.544	36.349	39.909	39.874	38.008	35.789	36.649	37.573	38.231	35.541	35.990	36.132	36.136	36.546	36.340	36.981	34.851	34.682	37.971	38.350	40.252	40.953	42.365	44.221	42.168	43.473	44.589	45.022	42.962	44.371	40.438	41.250	39.722	39.709	38.789	38.670	39.784				
50.337	51.539	51.741	52.915	52.697	53.171	49.021	48.561	48.430	47.140	46.715	45.281	44.122	43.003	43.980	44.808	43.430	41.720	42.707	41.559	46.045	45.223	45.004	44.999	43.918	46.205	46.325	47.777	48.057	48.131	49.629	45.092	46.222	46.464	45.975	44.926	44.817	46.439	45.737	43.903	43.149	43.069	43.301	43.686	43.653	42.203	41.955	40.554	39.810					
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
7.39	11.90	17.64	22.01	24.62	24.85	7.07	7.02	6.58	6.68	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.18	5.00	6.80	6.73	7.12	7.24	6.99	7.41	7.50	8.38	6.66	7.56	7.44	7.47	7.49	7.72	7.84	7.78	8.24	9.24	7.35	9.30	8.69	7.92	8.47	7.81	7.56	8.18	8.37	8.61	9.11	9.59				

1803	CE1	TYR	A	219	29.180	39.619	38.541	1.00	9.96	6	1803	ATOH	1856	CB	ASP	A	226	19.357	33.821	34.254	1.00	7.73	6
1804	CD2	TYR	A	219	28.416	37.404	40.008	1.00	9.35	6	1804	ATOH	1857	CG	ASP	A	226	18.559	35.071	33.990	1.00	7.95	6
1805	CE2	TYR	A	219	28.959	37.265	38.740	1.00	9.78	6	1805	ATOH	1858	OD1	ASP	A	226	17.512	35.272	34.681	1.00	10.67	8
1806	CZ	TYR	A	219	29.366	38.361	38.021	1.00	10.19	6	1806	ATOH	1859	OD2	ASP	A	226	18.962	35.869	33.172	1.00	7.61	8
1807	OH	TYR	A	219	29.899	38.187	36.757	1.00	11.08	8	1807	ATOH	1860	C	ASP	A	226	20.796	32.668	35.806	1.00	7.95	6
1808	C	TYR	A	219	25.279	39.259	41.447	1.00	8.69	6	1808	ATOH	1861	O	ASP	A	226	20.213	31.578	35.837	1.00	8.41	8
1809	O	TYR	A	219	24.836	39.946	40.527	1.00	8.37	8	1809	ATOH	1862	H	GLY	A	227	22.107	32.836	35.852	1.00	7.65	7
1810	H	ALA	A	220	24.676	38.131	41.869	1.00	9.13	7	1810	ATOH	1863	CA	GLY	A	227	22.992	31.679	35.946	1.00	7.46	6
1811	CA	ALA	A	220	23.427	37.644	41.267	1.00	9.77	6	1811	ATOH	1864	C	GLY	A	227	24.471	32.049	35.990	1.00	7.30	6
1812	CB	ALA	A	220	22.899	36.384	41.981	1.00	8.61	6	1812	ATOH	1865	O	GLY	A	227	24.880	33.197	36.042	1.00	6.95	8
1813	C	ALA	A	220	22.315	38.685	41.321	1.00	10.07	6	1813	ATOH	1866	H	PIE	A	228	25.294	30.990	36.029	1.00	7.33	7
1814	O	ALA	A	220	21.536	38.887	40.377	1.00	10.05	8	1814	ATOH	1867	CA	PIE	A	228	26.742	31.170	36.146	1.00	7.35	6
1815	H	ASH	A	221	22.192	39.338	42.473	1.00	10.39	7	1815	ATOH	1868	CB	PIE	A	228	27.220	30.898	37.558	1.00	6.74	6
1816	CA	ASH	A	221	21.200	40.374	42.757	1.00	10.66	6	1816	ATOH	1869	CG	PIE	A	228	26.640	31.708	38.672	1.00	9.48	6
1817	CB	ASH	A	221	21.013	40.698	44.262	1.00	13.90	6	1817	ATOH	1870	CD1	PIE	A	228	25.930	31.082	39.700	1.00	9.82	6
1818	CG	ASH	A	221	20.192	39.543	44.855	1.00	18.18	6	1818	ATOH	1871	CD2	PIE	A	228	26.800	33.097	38.702	1.00	8.78	6
1819	OD1	ASN	A	221	19.371	38.852	44.227	1.00	19.46	8	1819	ATOH	1872	CE1	PIE	A	228	25.415	31.869	40.731	1.00	10.75	6
1820	OD2	ASN	A	221	20.481	39.263	46.125	1.00	19.86	7	1820	ATOH	1873	CE2	PIE	A	228	26.277	33.860	39.746	1.00	9.42	6
1821	C	ASN	A	221	21.524	41.717	42.136	1.00	10.51	6	1821	ATOH	1874	CZ	PIE	A	228	25.590	33.241	40.786	1.00	9.64	6
1822	O	ASN	A	221	20.592	42.323	41.626	1.00	10.40	8	1822	ATOH	1875	C	PIE	A	228	27.603	30.229	35.304	1.00	7.29	6
1823	H	GLU	A	222	22.794	42.125	42.143	1.00	10.51	7	1823	ATOH	1876	O	PIE	A	228	27.245	29.086	34.995	1.00	7.76	8
1824	CA	GLU	A	222	23.160	43.432	41.552	1.00	10.18	6	1824	ATOH	1877	N	ARG	A	229	28.791	30.675	34.978	1.00	6.86	7
1825	CB	GLU	A	222	24.621	43.807	41.791	1.00	11.08	6	1825	ATOH	1878	CA	ARG	A	229	29.818	29.927	34.305	1.00	6.75	6
1826	CG	GLU	A	222	25.013	45.244	41.469	1.00	12.96	6	1826	ATOH	1879	CB	ARG	A	229	30.172	30.439	32.885	1.00	6.68	6
1827	CD	GLU	A	222	24.412	46.203	42.496	1.00	15.13	6	1827	ATOH	1880	CG	ARG	A	229	31.309	29.551	32.327	1.00	5.59	6
1828	OE1	GLU	A	222	23.947	45.777	43.576	1.00	15.79	8	1828	ATOH	1881	CD	ARG	A	229	32.646	30.283	32.584	1.00	7.41	6
1829	OE2	GLU	A	222	24.381	47.432	42.254	1.00	16.17	8	1829	ATOH	1882	NE	ARG	A	229	33.701	29.623	31.828	1.00	7.61	7
1830	C	GLU	A	222	22.903	43.428	40.052	1.00	9.82	6	1830	ATOH	1883	C2	ARG	A	229	34.985	29.905	31.872	1.00	8.29	6
1831	O	GLU	A	222	22.470	44.444	39.507	1.00	9.72	8	1831	ATOH	1884	NH1	ARG	A	229	35.833	29.189	31.139	1.00	7.90	7
1832	N	LEU	A	223	23.227	42.343	39.348	1.00	9.48	7	1832	ATOH	1885	NH2	ARG	A	229	35.388	30.913	32.626	1.00	7.66	7
1833	CA	LEU	A	223	23.009	42.319	37.909	1.00	9.43	6	1833	ATOH	1886	C	ARG	A	229	30.998	29.916	35.323	1.00	6.49	6
1834	CB	LEU	A	223	24.300	41.715	37.281	1.00	7.13	6	1834	ATOH	1887	O	ARG	A	229	31.518	30.980	35.697	1.00	6.39	8
1835	CG	LEU	A	223	25.595	42.503	37.476	1.00	5.72	6	1835	ATOH	1888	N	ILE	A	230	31.427	28.711	35.760	1.00	6.19	7
1836	CD1	LEU	A	223	26.752	41.715	36.835	1.00	5.00	6	1836	ATOH	1889	CA	ILE	A	230	32.530	28.667	36.752	1.00	5.82	6
1837	CD2	LEU	A	223	25.470	43.888	36.880	1.00	5.20	6	1837	ATOH	1890	CB	ILE	A	230	32.239	27.598	37.860	1.00	6.87	6
1838	C	LEU	A	223	21.794	41.550	37.456	1.00	9.44	6	1838	ATOH	1891	CG2	ILE	A	230	33.534	27.325	38.636	1.00	5.00	6
1839	O	LEU	A	223	21.561	41.335	36.280	1.00	9.57	8	1839	ATOH	1892	CG1	ILE	A	230	31.001	28.126	38.637	1.00	6.60	6
1840	N	SER	A	224	20.953	40.998	38.286	1.00	9.74	7	1840	ATOH	1893	CD1	ILE	A	230	30.470	27.073	39.606	1.00	11.75	6
1841	CA	SER	A	224	19.825	40.156	37.925	1.00	10.06	6	1841	ATOH	1894	C	ILE	A	230	33.907	28.409	36.148	1.00	5.56	6
1842	CB	SER	A	224	18.660	40.832	37.156	1.00	14.91	6	1842	ATOH	1895	O	ILE	A	230	34.225	27.368	35.555	1.00	5.42	8
1843	OG	SER	A	224	18.251	41.991	37.901	1.00	19.93	8	1843	ATOH	1896	H	ASP	A	231	34.758	29.428	36.246	1.00	5.02	7
1844	C	SER	A	224	20.293	38.979	37.047	1.00	9.76	6	1844	ATOH	1897	CA	ASP	A	231	36.086	29.322	35.714	1.00	5.00	6
1845	O	SER	A	224	19.648	38.752	36.004	1.00	9.74	8	1845	ATOH	1898	CB	ASP	A	231	36.693	30.746	35.684	1.00	5.00	6
1846	H	LEU	A	225	21.360	38.248	37.445	1.00	9.20	7	1846	ATOH	1899	CG	ASP	A	231	38.078	30.857	35.062	1.00	5.00	6
1847	CA	LEU	A	225	21.770	37.113	36.651	1.00	8.94	6	1847	ATOH	1900	OD1	ASP	A	231	38.156	30.584	33.864	1.00	5.00	8
1848	CB	LEU	A	225	23.164	36.688	37.088	1.00	10.36	6	1848	ATOH	1901	OD2	ASP	A	231	39.013	31.237	35.828	1.00	5.00	8
1849	CG	LEU	A	225	24.297	37.738	36.958	1.00	11.62	6	1849	ATOH	1902	C	ASP	A	231	37.016	28.427	36.518	1.00	5.00	6
1850	CD1	LEU	A	225	25.552	37.149	37.597	1.00	10.68	6	1850	ATOH	1903	O	ASP	A	231	36.987	28.462	37.750	1.00	5.00	8
1851	CD2	LEU	A	225	24.524	38.163	35.508	1.00	10.53	6	1851	ATOH	1904	N	ALA	A	232	37.861	27.681	35.819	1.00	5.00	7
1852	C	LEU	A	225	20.793	35.945	36.827	1.00	8.77	6	1852	ATOH	1905	CA	ALA	A	232	38.889	26.846	36.430	1.00	5.00	6
1853	O	LEU	A	225	20.084	35.785	37.796	1.00	8.44	8	1853	ATOH	1906	CB	ALA	A	232	39.030	27.869	36.945	1.00	6.65	6
1854	H	ASP	A	226	20.734	35.084	35.804	1.00	8.55	7	1854	ATOH	1907	C	ALA	A	232	38.515	25.954	37.593	1.00	5.00	6
1855	CA	ASP	A	226	19.950	33.911	35.674	1.00	7.98	6	1855	ATOH	1908	O	ALA	A	232	39.189	25.916	38.626	1.00	5.00	8

1909	ATOH	H	ALA A 233	37.399	25.223	37.414	1.00	5.00	7	1962	ATOH	CA	SER A 239	32.706	20.656	48.065	1.00	7.57	6
1910	ATOH	CA	ALA A 233	36.848	24.420	38.465	1.00	5.45	6	1963	ATOH	CB	SER A 239	32.940	19.984	49.417	1.00	7.79	6
1911	ATOH	CB	ALA A 233	35.529	23.866	37.899	1.00	6.05	6	1964	ATOH	OG	SER A 239	34.169	20.443	49.919	1.00	10.61	8
1912	ATOH	C	ALA A 233	37.755	23.310	38.952	1.00	6.00	6	1965	ATOH	C	SER A 239	32.410	22.159	48.249	1.00	7.33	6
1913	ATOH	O	ALA A 233	37.565	22.963	40.144	1.00	6.16	8	1966	ATOH	O	SER A 239	31.237	22.448	48.454	1.00	7.20	8
1914	ATOH	H	LYS A 234	38.683	22.764	38.169	1.00	5.81	7	1967	ATOH	H	PIE A 240	33.380	23.066	48.168	1.00	7.19	7
1915	ATOH	CA	LYS A 234	39.508	21.670	38.618	1.00	6.08	6	1968	ATOH	CA	PIE A 240	33.073	24.471	48.275	1.00	7.28	6
1916	ATOH	CB	LYS A 234	40.171	20.929	37.485	1.00	5.76	6	1969	ATOH	CB	PIE A 240	34.332	25.325	48.382	1.00	7.42	6
1917	ATOH	CG	LYS A 234	41.275	21.620	36.704	1.00	6.41	6	1970	ATOH	CG	PIE A 240	34.049	26.801	48.123	1.00	7.00	6
1918	ATOH	CD	LYS A 234	41.843	20.613	35.671	1.00	7.10	6	1971	ATOH	CD1	PIE A 240	33.390	27.560	49.085	1.00	6.31	6
1919	ATOH	CE	LYS A 234	43.118	21.208	34.994	1.00	5.42	6	1972	ATOH	CE2	PIE A 240	34.413	27.352	46.911	1.00	6.51	6
1920	ATOH	H2	LYS A 234	43.541	20.287	33.901	1.00	5.00	7	1973	ATOH	CE1	PIE A 240	33.091	28.886	48.775	1.00	7.11	6
1921	ATOH	C	LYS A 234	40.530	22.145	39.648	1.00	6.60	6	1974	ATOH	CE2	PIE A 240	34.116	28.674	46.615	1.00	5.97	6
1922	ATOH	O	LYS A 234	41.110	21.289	40.336	1.00	6.53	8	1975	ATOH	CZ	PIE A 240	33.479	29.440	47.555	1.00	5.18	6
1923	ATOH	H	HIS A 235	40.709	23.486	39.781	1.00	6.73	7	1976	ATOH	C	PIE A 240	32.259	24.900	47.044	1.00	7.56	6
1924	ATOH	CA	HIS A 235	41.640	23.999	40.796	1.00	6.75	6	1977	ATOH	O	PIE A 240	31.251	25.631	47.191	1.00	7.63	8
1925	ATOH	CB	HIS A 235	42.497	25.195	40.296	1.00	6.58	6	1978	ATOH	N	LEU A 241	32.639	24.464	45.838	1.00	7.46	7
1926	ATOH	CG	HIS A 235	43.030	24.789	38.959	1.00	6.14	6	1979	ATOH	CA	LEU A 241	31.880	24.877	44.661	1.00	7.91	6
1927	ATOH	CD2	HIS A 235	42.575	25.085	37.724	1.00	7.29	6	1980	ATOH	CB	LEU A 241	32.528	24.553	43.318	1.00	5.00	6
1928	ATOH	H01	HIS A 235	44.084	23.935	38.789	1.00	5.80	7	1981	ATOH	CG	LEU A 241	33.814	25.279	42.944	1.00	5.00	6
1929	ATOH	CE1	HIS A 235	44.290	23.756	37.502	1.00	7.11	6	1982	ATOH	CD1	LEU A 241	34.520	24.613	41.753	1.00	5.00	6
1930	ATOH	H2	HIS A 235	43.386	24.446	36.829	1.00	6.22	7	1983	ATOH	CD2	LEU A 241	33.548	26.754	42.654	1.00	5.00	6
1931	ATOH	C	HIS A 235	40.857	24.459	42.002	1.00	6.76	6	1984	ATOH	C	LEU A 241	30.418	24.377	44.720	1.00	8.46	6
1932	ATOH	O	HIS A 235	41.512	25.042	42.814	1.00	6.54	8	1985	ATOH	O	LEU A 241	29.483	25.127	44.303	1.00	8.58	8
1933	ATOH	H	ILE A 236	39.583	24.341	42.255	1.00	6.68	7	1986	ATOH	N	ARG A 242	30.184	23.164	45.219	1.00	8.61	7
1934	ATOH	CA	ILE A 236	38.916	24.866	43.434	1.00	6.87	6	1987	ATOH	CA	ARG A 242	28.777	22.774	45.286	1.00	8.92	6
1935	ATOH	CB	ILE A 236	37.858	25.949	43.026	1.00	5.00	6	1988	ATOH	CB	ARG A 242	28.716	21.286	45.431	1.00	10.58	6
1936	ATOH	CD2	ILE A 236	37.089	26.450	44.213	1.00	5.00	6	1989	ATOH	CG	ARG A 242	28.819	20.546	46.608	1.00	12.57	6
1937	ATOH	CG1	ILE A 236	38.558	27.103	42.238	1.00	5.00	6	1990	ATOH	CO	ARG A 242	27.687	19.642	47.094	1.00	13.52	6
1938	ATOH	CD1	ILE A 236	37.601	27.999	41.485	1.00	5.00	6	1991	ATOH	HE	ARG A 242	28.192	19.629	48.476	1.00	15.26	7
1939	ATOH	C	ILE A 236	38.228	23.724	44.193	1.00	7.20	6	1992	ATOH	CZ	ARG A 242	28.955	18.913	49.256	1.00	17.48	6
1940	ATOH	O	ILE A 236	37.587	22.852	43.555	1.00	7.08	8	1993	ATOH	HN1	ARG A 242	29.464	17.761	48.866	1.00	19.52	7
1941	ATOH	H	LYS A 237	38.407	23.693	45.498	1.00	7.57	7	1994	ATOH	HN2	ARG A 242	29.303	19.285	50.505	1.00	18.04	7
1942	ATOH	CA	LYS A 237	37.831	22.688	46.424	1.00	7.74	6	1995	ATOH	C	ARG A 242	28.042	23.548	46.379	1.00	8.91	6
1943	ATOH	CB	LYS A 237	37.828	23.257	47.868	1.00	9.45	6	1996	ATOH	O	ARG A 242	26.891	23.909	46.129	1.00	8.59	8
1944	ATOH	CG	LYS A 237	37.355	22.233	48.831	1.00	12.16	6	1997	ATOH	N	ASP A 243	28.653	23.828	47.526	1.00	9.00	7
1945	ATOH	CD	LYS A 237	37.037	22.463	50.263	1.00	15.99	6	1998	ATOH	CA	ASP A 243	27.984	24.591	48.533	1.00	9.47	6
1946	ATOH	CE	LYS A 237	37.992	23.114	51.189	1.00	19.56	6	1999	ATOH	CB	ASP A 243	28.812	24.581	49.811	1.00	11.98	6
1947	ATOH	H2	LYS A 237	37.579	22.767	52.623	1.00	22.41	7	2000	ATOH	CG	ASP A 243	28.766	23.183	50.417	1.00	15.20	6
1948	ATOH	C	LYS A 237	36.425	22.314	45.956	1.00	7.39	6	2001	ATOH	CO1	ASP A 243	29.580	22.982	51.372	1.00	19.21	8
1949	ATOH	O	LYS A 237	35.561	23.187	45.849	1.00	6.92	8	2002	ATOH	CO2	ASP A 243	28.049	22.251	50.036	1.00	13.33	8
1950	ATOH	N	PIE A 238	36.210	21.062	45.551	1.00	7.45	7	2003	ATOH	C	ASP A 243	27.798	26.049	48.117	1.00	9.53	6
1951	ATOH	CA	PIE A 238	34.912	20.689	44.944	1.00	7.67	6	2004	ATOH	O	ASP A 243	26.797	26.664	48.539	1.00	9.54	8
1952	ATOH	CB	PIE A 238	34.921	19.232	44.425	1.00	8.77	6	2005	ATOH	N	TRP A 244	28.755	26.581	47.303	1.00	9.34	7
1953	ATOH	CG	PIE A 238	35.992	18.884	43.442	1.00	9.75	6	2006	ATOH	CA	TRP A 244	28.622	28.005	46.908	1.00	9.20	6
1954	ATOH	CD1	PIE A 238	36.688	19.851	43.716	1.00	10.39	6	2007	ATOH	CB	TRP A 244	29.862	28.511	46.195	1.00	7.34	6
1955	ATOH	CD2	PIE A 238	36.262	17.529	43.199	1.00	9.45	6	2008	ATOH	CG	TRP A 244	29.831	29.924	45.719	1.00	8.91	6
1956	ATOH	CE1	PIE A 238	37.638	19.448	41.787	1.00	9.12	6	2009	ATOH	CO2	TRP A 244	29.442	30.367	44.411	1.00	9.51	6
1957	ATOH	CE2	PIE A 238	37.220	17.125	42.292	1.00	8.83	6	2010	ATOH	CE2	TRP A 244	29.589	31.773	44.384	1.00	10.54	6
1958	ATOH	CZ	PIE A 238	37.882	18.097	41.562	1.00	9.31	6	2011	ATOH	CE3	TRP A 244	29.020	29.698	43.243	1.00	10.38	6
1959	ATOH	C	PIE A 238	33.694	20.870	45.841	1.00	7.61	6	2012	ATOH	CD1	TRP A 244	30.168	31.065	46.419	1.00	9.07	6
1960	ATOH	O	PIE A 238	32.666	21.356	45.350	1.00	7.47	8	2013	ATOH	NE1	TRP A 244	30.036	32.191	45.638	1.00	9.59	7
1961	ATOH	N	SER A 239	33.801	20.475	47.113	1.00	7.50	7	2014	ATOH	NE2	TRP A 244	29.289	32.524	43.219	1.00	9.81	6

ATOM	2015	C23	TRP	A	244	28.727	30.446	42.096	1.00	10.45	6	ATOM	2068	CA	ALA	A	251	19.029	33.029	48.862	1.00	16.06	6
ATOM	2016	CH2	TRP	A	244	28.862	31.859	42.106	1.00	9.71	6	ATOM	2069	CB	ALA	A	251	20.374	33.774	48.984	1.00	16.48	6
ATOM	2017	C	TRP	A	244	27.386	28.200	46.006	1.00	9.28	6	ATOM	2070	C	ALA	A	251	18.276	33.769	47.765	1.00	16.26	6
ATOM	2018	O	TRP	A	244	26.651	29.168	46.164	1.00	8.82	8	ATOM	2071	O	ALA	A	251	17.596	34.738	48.088	1.00	16.47	8
ATOM	2019	N	VAL	A	245	27.217	27.284	45.056	1.00	9.64	7	ATOM	2072	N	THR	A	252	18.343	33.433	46.476	1.00	16.21	7
ATOM	2020	CA	VAL	A	245	26.082	27.305	44.114	1.00	10.52	6	ATOM	2073	CA	THR	A	252	17.631	34.224	45.487	1.00	16.03	6
ATOM	2021	CB	VAL	A	245	26.108	26.185	43.039	1.00	12.05	6	ATOM	2074	CB	THR	A	252	18.462	34.328	44.189	1.00	13.96	6
ATOM	2022	CG1	VAL	A	245	24.832	26.113	42.198	1.00	13.84	6	ATOM	2075	CG1	THR	A	252	18.697	32.968	43.824	1.00	11.77	8
ATOM	2023	CG2	VAL	A	245	27.262	26.450	42.081	1.00	13.35	6	ATOM	2076	CG2	THR	A	252	19.776	35.060	44.281	1.00	12.34	6
ATOM	2024	C	VAL	A	245	24.722	27.203	44.853	1.00	10.63	6	ATOM	2077	C	THR	A	252	16.292	33.577	45.170	1.00	16.40	6
ATOM	2025	O	VAL	A	245	23.758	27.906	44.590	1.00	10.02	8	ATOM	2078	O	THR	A	252	15.441	34.281	44.670	1.00	16.40	8
ATOM	2026	N	GLN	A	246	24.745	26.269	45.790	1.00	11.30	7	ATOM	2079	N	GLY	A	253	16.139	32.267	45.429	1.00	16.68	7
ATOM	2027	CA	GLN	A	246	23.552	26.022	46.634	1.00	12.37	6	ATOM	2080	CA	GLY	A	253	14.955	31.502	45.148	1.00	16.75	6
ATOM	2028	CB	GLN	A	246	23.878	24.727	47.381	1.00	18.96	6	ATOM	2081	C	GLY	A	253	14.963	31.170	43.660	1.00	17.06	6
ATOM	2029	CG	GLN	A	246	22.737	24.176	48.214	1.00	27.47	6	ATOM	2082	O	GLY	A	253	13.985	30.602	43.167	1.00	17.16	8
ATOM	2030	CD	GLN	A	246	23.367	23.366	49.350	1.00	34.63	6	ATOM	2083	O	LYS	A	254	16.018	31.475	42.888	1.00	17.07	7
ATOM	2031	OE1	GLN	A	246	22.842	23.446	50.493	1.00	37.91	8	ATOM	2084	CA	LYS	A	254	16.045	31.196	41.437	1.00	16.76	6
ATOM	2032	HE2	GLN	A	246	24.476	22.642	49.028	1.00	36.61	7	ATOM	2085	CB	LYS	A	254	16.734	32.377	40.748	1.00	18.37	6
ATOM	2033	C	GLN	A	246	23.153	27.225	47.485	1.00	12.39	6	ATOM	2086	CG	LYS	A	254	16.007	33.685	40.568	1.00	21.23	6
ATOM	2034	O	GLN	A	246	21.970	27.561	47.531	1.00	12.22	8	ATOM	2087	CG	LYS	A	254	16.884	34.884	40.536	1.00	23.96	6
ATOM	2035	N	ALA	A	247	24.083	27.968	48.099	1.00	12.46	7	ATOM	2088	CE	LYS	A	254	17.330	35.674	39.332	1.00	25.51	6
ATOM	2036	CA	ALA	A	247	23.852	29.144	48.893	1.00	12.61	6	ATOM	2089	NZ	LYS	A	254	18.369	36.723	39.792	1.00	27.00	7
ATOM	2037	CB	ALA	A	247	25.094	29.791	49.517	1.00	12.74	6	ATOM	2090	C	LYS	A	254	16.731	29.871	41.097	1.00	16.34	6
ATOM	2038	C	ALA	A	247	23.231	30.263	48.050	1.00	12.74	6	ATOM	2091	O	LYS	A	254	17.533	29.323	41.896	1.00	16.45	8
ATOM	2039	O	ALA	A	247	22.308	30.857	48.561	1.00	12.85	8	ATOM	2092	N	GLU	A	255	16.459	29.313	39.928	1.00	15.71	7
ATOM	2040	N	VAL	A	248	23.710	30.495	46.838	1.00	12.75	7	ATOM	2093	CA	GLU	A	255	17.084	28.072	39.466	1.00	15.30	6
ATOM	2041	CA	VAL	A	248	23.159	31.471	45.933	1.00	12.69	6	ATOM	2094	CB	GLU	A	255	16.504	27.668	38.102	1.00	18.71	6
ATOM	2042	CB	VAL	A	248	24.009	31.688	44.684	1.00	11.87	6	ATOM	2095	CG	GLU	A	255	16.954	26.337	37.542	1.00	24.80	6
ATOM	2043	CG1	VAL	A	248	23.357	32.721	43.754	1.00	12.19	6	ATOM	2096	CD	GLU	A	255	16.927	26.270	36.020	1.00	29.50	6
ATOM	2044	CG2	VAL	A	248	25.400	32.171	45.014	1.00	11.42	6	ATOM	2097	OE1	GLU	A	255	16.083	26.965	35.393	1.00	31.45	8
ATOM	2045	C	VAL	A	248	21.748	31.040	45.537	1.00	12.91	6	ATOM	2098	OE2	GLU	A	255	17.730	25.553	35.340	1.00	31.98	8
ATOM	2046	O	VAL	A	248	20.866	31.889	45.506	1.00	12.81	8	ATOM	2099	C	GLU	A	255	18.623	28.183	39.365	1.00	14.27	6
ATOM	2047	N	ARG	A	249	21.403	29.791	45.237	1.00	13.31	7	ATOM	2100	O	GLU	A	255	19.417	27.324	39.733	1.00	14.14	8
ATOM	2048	CA	ARG	A	249	20.124	29.352	44.897	1.00	13.92	6	ATOM	2101	N	MET	A	256	19.098	29.303	38.859	1.00	13.25	7
ATOM	2049	CB	ARG	A	249	20.066	27.906	44.404	1.00	11.75	6	ATOM	2102	CA	MET	A	256	20.476	29.628	38.676	1.00	12.49	6
ATOM	2050	CG	ARG	A	249	20.681	27.726	43.033	1.00	12.59	6	ATOM	2103	CB	MET	A	256	21.171	29.970	39.998	1.00	12.38	6
ATOM	2051	CD	ARG	A	249	20.814	26.274	42.576	1.00	12.82	6	ATOM	2104	CG	MET	A	256	20.740	31.237	40.705	1.00	13.41	6
ATOM	2052	HE	ARG	A	249	21.411	26.198	41.224	1.00	13.02	7	ATOM	2105	SD	MET	A	256	20.539	32.774	39.751	1.00	13.00	16
ATOM	2053	CZ	ARG	A	249	22.045	25.141	40.739	1.00	13.82	6	ATOM	2106	CE	MET	A	256	22.245	33.221	39.432	1.00	12.60	6
ATOM	2054	HI1	ARG	A	249	22.150	24.041	41.476	1.00	11.68	7	ATOM	2107	C	MET	A	256	21.209	28.486	37.966	1.00	11.87	6
ATOM	2055	HI2	ARG	A	249	22.589	25.166	39.515	1.00	15.22	7	ATOM	2108	O	MET	A	256	22.065	27.824	38.595	1.00	10.99	8
ATOM	2056	C	ARG	A	249	19.215	29.503	46.125	1.00	14.55	6	ATOM	2109	N	PIE	A	257	20.904	28.261	36.696	1.00	10.24	6
ATOM	2057	O	ARG	A	249	18.082	30.005	45.970	1.00	14.34	8	ATOM	2110	CA	PIE	A	257	21.612	27.238	35.914	1.00	9.31	6
ATOM	2058	N	GLU	A	250	19.685	29.106	47.329	1.00	15.16	7	ATOM	2111	CB	PIE	A	257	21.254	27.347	34.397	1.00	9.08	6
ATOM	2059	CA	GLU	A	250	18.794	29.252	48.498	1.00	15.83	6	ATOM	2112	CG	PIE	A	257	22.056	26.339	33.591	1.00	9.08	6
ATOM	2060	CB	GLU	A	250	19.437	28.816	49.790	1.00	21.15	6	ATOM	2113	CD1	PIE	A	257	21.634	25.032	33.491	1.00	7.86	6
ATOM	2061	CG	GLU	A	250	18.902	27.566	50.460	1.00	28.24	6	ATOM	2114	CD2	PIE	A	257	23.248	26.741	32.991	1.00	8.44	6
ATOM	2062	CD	GLU	A	250	20.067	26.619	50.807	1.00	32.12	6	ATOM	2115	CE1	PIE	A	257	22.425	24.132	32.769	1.00	9.31	6
ATOM	2063	OE1	GLU	A	250	21.116	27.047	51.333	1.00	34.30	8	ATOM	2116	CE2	PIE	A	257	24.059	25.861	32.292	1.00	9.08	6
ATOM	2064	HE2	GLU	A	250	19.907	25.331	50.478	1.00	32.80	7	ATOM	2117	CZ	PIE	A	257	23.624	24.537	32.171	1.00	10.03	6
ATOM	2065	C	GLN	A	250	18.362	30.699	48.707	1.00	15.86	6	ATOM	2118	C	PIE	A	257	23.115	27.439	36.047	1.00	9.70	6
ATOM	2066	O	GLN	A	250	17.196	31.022	48.871	1.00	15.83	8	ATOM	2119	O	PIE	A	257	23.583	28.593	35.876	1.00	9.75	8
ATOM	2067	N	ALA	A	251	19.316	31.621	48.689	1.00	15.85	7	ATOM	2120	N	THR	A	258	23.933	26.447	36.329	1.00	9.20	7

ATOH	2121	CA	THR A 258	25.392	26.609	36.450	1.00	8.71	6	ATOH	2174	N	GLN A 264	39.758	18.950	31.301	1.00	10.57	7
ATOH	2122	CB	THR A 258	25.824	26.583	37.938	1.00	8.83	6	ATOH	2175	CA	GLN A 264	40.441	17.687	31.185	1.00	10.92	6
ATOH	2123	OG1	THR A 258	25.203	27.678	38.617	1.00	7.38	8	ATOH	2176	CB	GLN A 264	40.619	16.999	32.536	1.00	14.66	6
ATOH	2124	CG2	THR A 258	27.337	26.720	38.142	1.00	8.42	6	ATOH	2177	CG	GLN A 264	41.796	16.043	32.600	1.00	18.65	6
ATOH	2125	C	THR A 258	26.136	25.533	35.646	1.00	8.29	6	ATOH	2178	CD	GLN A 264	41.972	15.344	33.934	1.00	22.60	6
ATOH	2126	O	THR A 258	25.764	24.341	35.606	1.00	8.22	8	ATOH	2179	OE1	GLN A 264	41.214	15.481	34.907	1.00	24.23	8
ATOH	2127	N	VAL A 259	27.160	25.972	34.922	1.00	7.82	7	ATOH	2180	NE2	GLN A 264	42.996	14.478	34.047	1.00	23.90	7
ATOH	2128	CA	VAL A 259	28.001	25.077	34.102	1.00	7.47	6	ATOH	2181	C	GLN A 264	39.681	16.811	30.191	1.00	11.04	6
ATOH	2129	CB	VAL A 259	27.859	25.175	32.564	1.00	5.00	6	ATOH	2182	O	GLN A 264	38.461	16.643	30.232	1.00	10.83	8
ATOH	2130	CG1	VAL A 259	28.101	26.589	32.036	1.00	5.00	6	ATOH	2183	N	ASN A 265	40.454	16.216	29.289	1.00	11.25	7
ATOH	2131	CG2	VAL A 259	28.799	24.202	31.809	1.00	5.00	6	ATOH	2184	CA	ASN A 265	40.151	15.322	28.209	1.00	11.87	6
ATOH	2132	C	VAL A 259	29.428	25.381	34.552	1.00	7.58	6	ATOH	2185	CB	ASN A 265	41.223	15.365	27.078	1.00	11.52	6
ATOH	2133	O	VAL A 259	29.821	26.552	34.634	1.00	7.78	8	ATOH	2186	CG	ASN A 265	40.655	14.637	25.854	1.00	12.03	6
ATOH	2134	N	ALA A 260	30.181	24.348	34.913	1.00	7.84	7	ATOH	2187	OO1	ASN A 265	39.485	14.278	25.764	1.00	11.79	8
ATOH	2135	CA	ALA A 260	31.555	24.487	35.346	1.00	8.08	6	ATOH	2188	MO2	ASN A 265	41.445	14.294	24.857	1.00	11.74	7
ATOH	2136	CD	ALA A 260	31.962	23.621	36.534	1.00	7.64	6	ATOH	2189	C	ASN A 265	40.028	13.873	28.691	1.00	12.36	6
ATOH	2137	C	ALA A 260	32.523	24.076	34.215	1.00	8.28	6	ATOH	2190	O	ASN A 265	40.755	13.007	28.282	1.00	12.25	8
ATOH	2138	O	ALA A 260	32.266	23.091	33.536	1.00	8.26	8	ATOH	2191	N	ASN A 266	39.116	13.676	29.634	1.00	13.06	7
ATOH	2139	N	GLU A 261	33.579	24.848	34.057	1.00	8.60	7	ATOH	2192	CA	ASN A 266	38.844	12.428	30.337	1.00	13.75	6
ATOH	2140	CA	GLU A 261	34.628	24.574	33.125	1.00	8.60	6	ATOH	2193	CB	ASN A 266	39.910	12.362	31.416	1.00	18.58	6
ATOH	2141	CB	GLU A 261	35.346	25.828	32.600	1.00	11.43	6	ATOH	2194	CG	ASN A 266	40.150	11.016	32.031	1.00	22.56	6
ATOH	2142	CG	GLU A 261	36.281	25.350	31.518	1.00	17.13	6	ATOH	2195	OO1	ASN A 266	41.311	10.519	31.969	1.00	26.43	8
ATOH	2143	CD	GLU A 261	36.823	26.339	30.525	1.00	23.18	6	ATOH	2196	MO2	ASN A 266	39.160	10.410	32.662	1.00	21.13	7
ATOH	2144	OE1	GLU A 261	36.068	26.970	29.694	1.00	25.81	8	ATOH	2197	C	ASN A 266	37.441	12.394	30.944	1.00	13.73	6
ATOH	2145	OE2	GLU A 261	38.080	26.441	30.593	1.00	25.35	8	ATOH	2198	O	ASN A 266	37.161	13.123	31.927	1.00	13.68	8
ATOH	2146	C	GLU A 261	35.844	23.659	33.847	1.00	8.48	6	ATOH	2199	N	ALA A 267	36.552	11.545	30.362	1.00	13.47	7
ATOH	2147	O	GLU A 261	36.514	24.148	34.558	1.00	8.19	8	ATOH	2200	CA	ALA A 267	35.178	11.440	30.835	1.00	13.35	6
ATOH	2148	N	TYR A 262	35.578	22.360	33.730	1.00	8.54	7	ATOH	2201	CB	ALA A 267	34.330	10.522	29.944	1.00	12.56	6
ATOH	2149	CA	TYR A 262	36.500	21.387	34.293	1.00	8.87	6	ATOH	2202	C	ALA A 267	35.076	10.997	32.287	1.00	13.08	6
ATOH	2150	CB	TYR A 262	35.838	20.183	34.966	1.00	8.94	6	ATOH	2203	O	ALA A 267	34.195	11.454	33.027	1.00	13.14	8
ATOH	2151	CG	TYR A 262	36.761	19.321	35.821	1.00	9.11	6	ATOH	2204	N	GLY A 268	35.918	10.106	32.733	1.00	12.97	7
ATOH	2152	CD1	TYR A 262	36.660	19.322	37.206	1.00	9.01	6	ATOH	2205	CA	GLY A 268	35.973	9.564	34.083	1.00	12.93	6
ATOH	2153	CE1	TYR A 262	37.509	18.576	37.984	1.00	9.15	6	ATOH	2206	C	GLY A 268	36.184	10.653	35.146	1.00	13.05	6
ATOH	2154	CD2	TYR A 262	37.743	18.497	35.253	1.00	9.44	6	ATOH	2207	O	GLY A 268	35.512	10.656	36.213	1.00	13.01	8
ATOH	2155	CE2	TYR A 262	38.605	17.723	36.026	1.00	9.65	6	ATOH	2208	N	LYS A 269	37.109	11.575	34.879	1.00	12.90	7
ATOH	2156	CZ	TYR A 262	38.490	17.788	37.415	1.00	9.42	6	ATOH	2209	CA	LYS A 269	37.425	12.681	35.786	1.00	13.04	6
ATOH	2157	OH	TYR A 262	39.305	17.012	38.214	1.00	9.41	8	ATOH	2210	CB	LYS A 269	38.790	13.296	35.417	1.00	17.83	6
ATOH	2158	C	TYR A 262	37.424	20.977	33.104	1.00	8.97	6	ATOH	2211	CG	LYS A 269	39.840	12.506	36.217	1.00	22.85	6
ATOH	2159	O	TYR A 262	37.008	20.107	32.297	1.00	9.09	8	ATOH	2212	CD	LYS A 269	40.869	12.034	35.211	1.00	27.74	6
ATOH	2160	N	TRP A 263	38.590	21.592	32.945	1.00	9.15	7	ATOH	2213	CE	LYS A 269	41.722	10.885	35.785	1.00	30.85	6
ATOH	2161	CA	TRP A 263	39.403	21.292	31.774	1.00	9.76	6	ATOH	2214	NZ	LYS A 269	42.663	10.356	34.698	1.00	32.23	7
ATOH	2162	CB	TRP A 263	40.183	22.560	31.346	1.00	9.45	6	ATOH	2215	C	LYS A 269	36.296	13.699	35.776	1.00	12.76	6
ATOH	2163	CG	TRP A 263	40.638	22.366	29.917	1.00	11.66	6	ATOH	2216	O	LYS A 269	35.918	14.230	36.828	1.00	12.65	8
ATOH	2164	CD2	TRP A 263	39.892	22.703	28.733	1.00	12.75	6	ATOH	2217	N	LEU A 270	35.696	13.903	34.596	1.00	12.42	7
ATOH	2165	CE2	TRP A 263	40.662	22.299	27.612	1.00	13.78	6	ATOH	2218	CA	LEU A 270	34.539	14.810	34.538	1.00	12.16	6
ATOH	2166	CE3	TRP A 263	38.631	23.289	28.512	1.00	12.04	6	ATOH	2219	CB	LEU A 270	34.164	15.161	33.088	1.00	13.49	6
ATOH	2167	CD1	TRP A 263	41.800	21.810	29.466	1.00	12.57	6	ATOH	2220	CG	LEU A 270	34.959	16.348	32.467	1.00	13.12	6
ATOH	2168	NE1	TRP A 263	41.820	21.731	28.078	1.00	13.80	7	ATOH	2221	CD1	LEU A 270	34.614	17.623	33.197	1.00	13.42	6
ATOH	2169	C22	TRP A 263	40.205	22.513	26.299	1.00	14.12	6	ATOH	2222	CD2	LEU A 270	36.465	16.210	32.550	1.00	13.72	6
ATOH	2170	C23	TRP A 263	38.201	23.453	27.210	1.00	10.77	6	ATOH	2223	C	LEU A 270	33.412	14.169	35.315	1.00	11.76	6
ATOH	2171	CH2	TRP A 263	38.970	23.094	26.122	1.00	11.88	6	ATOH	2224	O	LEU A 270	32.700	14.934	35.981	1.00	11.63	8
ATOH	2172	C	TRP A 263	40.303	20.053	31.833	1.00	10.24	6	ATOH	2225	N	GLU A 271	33.219	12.851	35.281	1.00	11.41	7
ATOH	2173	O	TRP A 263	41.436	20.018	32.294	1.00	10.30	8	ATOH	2226	CA	GLU A 271	33.136	12.233	36.051	1.00	11.29	6

2227	ATOH	CB	GLU A 271	32.024	10.817	35.510	1.00	16.08	6	6	2280	CA	THR A 277	29.173	18.187	43.406	1.00	12.78	6
2228	ATOH	CG	GLU A 271	31.015	10.010	36.333	1.00	23.09	6	6	2281	CB	THR A 277	29.520	19.264	42.357	1.00	12.02	6
2229	ATOH	CD	GLU A 271	30.861	8.627	35.720	1.00	27.19	6	6	2282	OG1	THR A 277	29.323	18.649	41.065	1.00	12.30	8
2230	ATOH	OE1	GLU A 271	29.716	8.351	35.359	1.00	29.23	8	6	2283	CG2	THR A 277	30.941	19.791	42.492	1.00	8.90	6
2231	ATOH	OE2	GLU A 271	31.830	7.845	35.526	1.00	30.01	8	6	2284	C	THR A 277	27.701	17.794	43.416	1.00	12.70	6
2232	ATOH	C	GLU A 271	32.339	12.279	37.554	1.00	10.89	6	6	2285	O	THR A 277	26.812	18.613	43.190	1.00	12.66	8
2233	ATOH	O	GLU A 271	31.458	12.370	38.404	1.00	10.58	8	6	2286	H	SER A 278	27.426	16.518	43.673	1.00	12.73	7
2234	ATOH	ASH A 272	33.615	12.189	37.987	1.00	10.66	7	6	2287	CA	SER A 278	26.069	16.047	43.729	1.00	12.83	6	
2235	ATOH	ASH A 272	34.008	12.309	39.385	1.00	10.31	6	6	2288	CB	SER A 278	25.280	16.804	44.854	1.00	18.04	8	
2236	ATOH	CB	ASH A 272	35.520	12.089	39.643	1.00	11.32	6	6	2289	OG	SER A 278	25.963	16.531	46.061	1.00	14.69	6
2237	ATOH	CG	ASH A 272	35.969	12.380	41.064	1.00	11.99	6	6	2290	C	SER A 278	25.283	16.294	42.474	1.00	12.85	6
2238	ATOH	OO1	ASH A 272	35.616	11.603	41.966	1.00	11.66	8	6	2291	O	SER A 278	24.049	16.483	42.663	1.00	13.07	8
2239	ATOH	OO2	ASH A 272	36.701	13.474	41.322	1.00	12.45	7	6	2292	N	PIE A 279	25.774	16.339	41.260	1.00	12.49	7
2240	ATOH	C	ASH A 272	33.588	13.709	39.873	1.00	9.78	6	6	2293	CA	PIE A 279	24.897	16.593	40.100	1.00	12.16	6
2241	ATOH	O	ASH A 272	33.080	13.897	40.979	1.00	9.63	8	6	2294	CB	PIE A 279	23.976	15.344	39.973	1.00	12.70	6
2242	ATOH	H	TYR A 273	33.777	14.748	39.063	1.00	9.45	7	6	2295	CG	PIE A 279	24.772	14.122	39.524	1.00	12.87	6
2243	ATOH	CA	TYR A 273	33.369	16.104	39.486	1.00	9.06	6	6	2296	CD1	PIE A 279	25.183	13.153	40.435	1.00	13.85	6
2244	ATOH	CB	TYR A 273	33.908	17.179	38.558	1.00	8.65	6	6	2297	CD2	PIE A 279	25.005	13.919	38.199	1.00	13.30	6
2245	ATOH	CG	TYR A 273	33.509	18.626	38.903	1.00	8.44	6	6	2298	CE1	PIE A 279	25.903	12.038	40.045	1.00	13.14	6
2246	ATOH	OO1	TYR A 273	34.242	19.333	39.838	1.00	8.51	6	6	2299	CE2	PIE A 279	25.801	12.799	37.786	1.00	13.99	6
2247	ATOH	CE1	TYR A 273	33.915	20.650	40.228	1.00	8.39	6	6	2300	CZ	PIE A 279	26.246	11.878	38.726	1.00	13.30	6
2248	ATOH	CD2	TYR A 273	32.391	19.231	38.364	1.00	8.33	6	6	2301	C	PIE A 279	24.170	17.912	40.149	1.00	12.03	6
2249	ATOH	CE2	TYR A 273	32.015	20.523	38.695	1.00	8.66	6	6	2302	O	PIE A 279	23.185	18.072	40.882	1.00	12.27	8
2250	ATOH	CZ	TYR A 273	32.827	21.214	39.625	1.00	8.60	6	6	2303	N	ASN A 280	24.646	18.942	40.984	1.00	11.58	7
2251	ATOH	OH	TYR A 273	32.452	22.481	39.938	1.00	8.94	8	6	2304	CA	ASN A 280	23.979	20.228	40.984	1.00	11.30	6
2252	ATOH	C	TYR A 273	31.837	16.135	39.662	1.00	9.06	6	6	2305	CB	ASN A 280	24.025	20.735	42.438	1.00	11.18	6
2253	ATOH	O	TYR A 273	31.340	16.679	40.688	1.00	8.80	8	6	2306	CG	ASN A 280	25.222	21.558	42.868	1.00	13.48	6
2254	ATOH	H	LEU A 274	31.061	15.569	38.736	1.00	9.52	7	6	2307	OO1	ASN A 280	26.142	21.809	42.087	1.00	12.89	8
2255	ATOH	CA	LEU A 274	29.590	15.550	38.849	1.00	10.16	6	6	2308	ND2	ASN A 280	25.289	22.094	44.111	1.00	12.18	7
2256	ATOH	CB	LEU A 274	28.901	14.856	37.646	1.00	10.22	6	6	2309	C	ASN A 280	24.422	21.247	39.927	1.00	10.94	6
2257	ATOH	CG	LEU A 274	29.158	15.528	36.280	1.00	10.91	6	6	2310	O	ASN A 280	23.910	22.353	39.820	1.00	11.03	8
2258	ATOH	CD1	LEU A 274	28.719	14.634	35.107	1.00	11.67	6	6	2311	N	GLN A 281	25.325	20.890	39.032	1.00	10.60	7
2259	ATOH	CD2	LEU A 274	28.432	16.843	36.198	1.00	10.03	6	6	2312	CA	GLN A 281	25.784	21.736	37.949	1.00	10.04	6
2260	ATOH	C	LEU A 274	29.157	14.918	40.173	1.00	10.59	6	6	2313	CB	GLN A 281	26.930	22.636	38.400	1.00	9.98	6
2261	ATOH	O	LEU A 274	28.353	15.463	40.920	1.00	10.27	8	6	2314	CG	GLN A 281	28.117	21.977	39.038	1.00	9.72	6
2262	ATOH	H	ASH A 275	29.706	13.730	40.471	1.00	11.45	7	6	2315	CD	GLN A 281	29.055	22.863	39.859	1.00	9.00	6
2263	ATOH	CA	ASH A 275	29.463	13.009	41.709	1.00	12.37	6	6	2316	OE1	GLN A 281	30.064	23.342	39.350	1.00	8.97	8
2264	ATOH	CB	ASH A 275	30.287	11.694	41.835	1.00	19.11	6	6	2317	NE2	GLN A 281	28.835	23.085	41.151	1.00	8.05	7
2265	ATOH	CG	ASH A 275	29.761	10.565	40.962	1.00	24.07	6	6	2318	C	GLN A 281	26.239	20.871	36.771	1.00	9.46	6
2266	ATOH	OO1	ASH A 275	28.743	9.915	41.314	1.00	27.53	8	6	2319	O	GLN A 281	26.615	19.703	36.902	1.00	9.22	8
2267	ATOH	OO2	ASH A 275	30.352	10.254	39.805	1.00	25.40	7	6	2320	H	SER A 282	26.224	21.522	35.616	1.00	9.14	7
2268	ATOH	C	ASH A 275	29.820	13.870	42.924	1.00	12.34	6	6	2321	CA	SER A 282	26.674	20.851	34.389	1.00	8.74	6
2269	ATOH	O	ASH A 275	28.964	14.072	43.761	1.00	12.19	8	6	2322	CB	SER A 282	25.985	21.419	33.131	1.00	7.22	6
2270	ATOH	H	LYS A 276	31.008	14.435	43.005	1.00	12.51	7	6	2323	OG	SER A 282	24.607	21.123	33.102	1.00	6.53	8
2271	ATOH	CA	LYS A 276	31.461	15.251	44.130	1.00	12.99	6	6	2324	C	SER A 282	28.170	21.077	34.201	1.00	8.54	6
2272	ATOH	CB	LYS A 276	32.952	15.605	44.000	1.00	12.82	6	6	2325	O	SER A 282	28.773	21.913	34.919	1.00	8.89	8
2273	ATOH	CG	LYS A 276	33.825	14.346	44.050	1.00	13.95	6	6	2326	H	VAL A 283	28.777	20.420	33.240	1.00	8.11	7
2274	ATOH	CD	LYS A 276	33.535	13.485	45.269	1.00	14.29	6	6	2327	CA	VAL A 283	30.154	20.596	32.841	1.00	7.98	6
2275	ATOH	CE	LYS A 276	34.141	12.103	45.203	1.00	13.18	6	6	2328	CB	VAL A 283	31.137	19.443	33.210	1.00	8.54	6
2276	ATOH	NZ	LYS A 276	35.602	12.070	44.906	1.00	13.50	7	6	2329	CG1	VAL A 283	31.457	19.441	34.708	1.00	9.20	6
2277	ATOH	C	LYS A 276	30.651	16.533	44.311	1.00	13.24	6	6	2330	CG2	VAL A 283	30.599	18.117	32.719	1.00	7.85	6
2278	ATOH	O	LYS A 276	30.650	17.117	45.412	1.00	13.75	8	6	2331	C	VAL A 283	30.218	20.758	31.304	1.00	7.87	6
2279	ATOH	H	THR A 277	29.966	16.979	43.256	1.00	12.99	7	6	2332	O	VAL A 283	29.342	20.265	30.572	1.00	7.75	8

2333	ATOH	H	PIE A 284	31.212	21.483	30.801	1.00	7.72	7
2334	ATOH	CA	PIE A 284	31.460	21.589	29.383	1.00	7.67	6
2335	ATOH	CB	PIE A 284	32.518	22.649	29.110	1.00	7.48	6
2336	ATOH	CG	PIE A 284	31.953	24.040	29.240	1.00	7.61	6
2337	ATOH	CD1	PIE A 284	32.301	24.886	30.277	1.00	6.90	6
2338	ATOH	CD2	PIE A 284	31.062	24.475	28.252	1.00	7.80	6
2339	ATOH	CE1	PIE A 284	31.782	26.167	30.312	1.00	8.33	6
2340	ATOH	CE2	PIE A 284	30.501	25.756	28.282	1.00	6.48	6
2341	ATOH	CZ	PIE A 284	30.882	26.602	29.314	1.00	7.74	6
2342	ATOH	C	PIE A 284	31.997	20.212	28.924	1.00	7.86	6
2343	ATOH	C	PIE A 284	32.833	19.541	29.627	1.00	7.99	7
2344	ATOH	H	ASP A 285	31.517	19.758	27.741	1.00	7.99	7
2345	ATOH	CA	ASP A 285	31.997	18.452	27.212	1.00	8.11	6
2346	ATOH	CA	ASP A 285	30.919	17.867	26.269	1.00	8.64	6
2347	ATOH	CG	ASP A 285	31.063	16.361	26.096	1.00	9.93	6
2348	ATOH	CG	ASP A 285	32.173	15.774	26.289	1.00	8.07	8
2349	ATOH	CG	ASP A 285	30.026	15.731	25.769	1.00	9.24	8
2350	ATOH	C	ASP A 285	33.339	18.591	26.496	1.00	8.25	6
2351	ATOH	C	ASP A 285	33.394	18.729	25.236	1.00	8.58	8
2352	ATOH	H	VAL A 286	34.468	18.590	27.218	1.00	7.95	7
2353	ATOH	CA	VAL A 286	35.813	18.709	26.644	1.00	7.75	6
2354	ATOH	CA	VAL A 286	36.851	18.934	27.764	1.00	7.80	6
2355	ATOH	CG1	VAL A 286	38.270	19.085	27.261	1.00	5.55	6
2356	ATOH	CG2	VAL A 286	36.418	20.221	28.524	1.00	8.40	6
2357	ATOH	C	VAL A 286	36.145	17.549	25.719	1.00	7.74	6
2358	ATOH	O	VAL A 286	36.611	17.833	24.601	1.00	7.94	8
2359	ATOH	H	PRO A 287	35.967	16.276	26.097	1.00	7.41	7
2360	ATOH	CD	PRO A 287	35.495	15.854	27.413	1.00	7.11	6
2361	ATOH	CA	PRO A 287	36.262	15.131	25.226	1.00	7.24	6
2362	ATOH	CA	PRO A 287	35.802	13.885	25.970	1.00	7.14	6
2363	ATOH	CG	PRO A 287	35.741	14.357	27.396	1.00	7.12	6
2364	ATOH	C	PRO A 287	35.589	15.313	23.873	1.00	7.43	6
2365	ATOH	O	PRO A 287	36.214	15.113	22.834	1.00	7.51	8
2366	ATOH	H	LEU A 288	34.293	15.681	23.762	1.00	7.47	7
2367	ATOH	CA	LEU A 288	33.608	15.904	22.504	1.00	7.34	6
2368	ATOH	CB	LEU A 288	32.149	16.325	22.654	1.00	7.25	6
2369	ATOH	CG	LEU A 288	31.384	15.185	20.494	1.00	8.35	6
2370	ATOH	CD1	LEU A 288	31.430	16.481	21.283	1.00	8.34	6
2371	ATOH	CD2	LEU A 288	30.038	16.988	21.510	1.00	5.28	6
2372	ATOH	C	LEU A 288	34.329	16.998	21.722	1.00	7.39	6
2373	ATOH	O	LEU A 288	34.308	16.793	20.525	1.00	7.49	8
2374	ATOH	H	HIS A 289	34.847	18.097	22.260	1.00	7.34	7
2375	ATOH	CA	HIS A 289	35.583	19.114	21.525	1.00	7.21	6
2376	ATOH	CB	HIS A 289	36.094	20.260	22.425	1.00	5.61	6
2377	ATOH	CG	HIS A 289	37.215	21.083	21.852	1.00	5.00	6
2378	ATOH	CD2	HIS A 289	38.548	21.040	22.012	1.00	5.00	6
2379	ATOH	CD1	HIS A 289	36.986	22.086	20.914	1.00	5.00	6
2380	ATOH	CE1	HIS A 289	38.127	22.570	20.527	1.00	5.00	7
2381	ATOH	CE2	HIS A 289	39.124	21.983	21.176	1.00	5.00	6
2382	ATOH	C	HIS A 289	36.776	18.507	20.805	1.00	7.52	6
2383	ATOH	O	HIS A 289	37.083	18.809	19.647	1.00	7.41	8
2384	ATOH	H	PIE A 290	37.518	17.654	21.545	1.00	7.75	7
2385	ATOH	CA	PIE A 290	38.721	16.971	21.050	1.00	8.12	6
2386	ATOH	CB	PIE A 290	39.575	16.332	22.175	1.00	7.08	6
2387	ATOH	CG	PIE A 290	40.370	17.378	22.893	1.00	7.95	6
2388	ATOH	CD1	PIE A 290	40.054	17.819	24.152	1.00	7.13	6
2389	ATOH	CD2	PIE A 290	41.431	18.012	22.214	1.00	9.46	6
2390	ATOH	CE1	PIE A 290	40.764	18.810	24.791	1.00	8.24	6
2391	ATOH	CE2	PIE A 290	42.137	19.075	22.838	1.00	9.38	6
2392	ATOH	CZ	PIE A 290	41.830	19.458	24.125	1.00	9.13	6
2393	ATOH	C	PIE A 290	38.361	15.943	19.984	1.00	8.42	6
2394	ATOH	O	PIE A 290	39.158	15.881	19.025	1.00	8.61	8
2395	ATOH	N	ASN A 291	37.239	15.234	20.127	1.00	8.43	7
2396	ATOH	CA	ASN A 291	36.826	14.303	19.077	1.00	8.66	6
2397	ATOH	CB	ASN A 291	35.581	13.461	19.414	1.00	9.01	6
2398	ATOH	CG	ASN A 291	35.866	12.427	20.505	1.00	10.93	6
2399	ATOH	CG1	ASN A 291	37.040	12.332	20.954	1.00	10.93	6
2400	ATOH	CG2	ASN A 291	34.848	11.690	20.917	1.00	8.51	7
2401	ATOH	C	ASN A 291	36.507	15.080	17.798	1.00	8.93	6
2402	ATOH	O	ASN A 291	36.824	14.630	16.701	1.00	8.32	8
2403	ATOH	N	LEU A 292	35.808	16.219	17.925	1.00	9.66	7
2404	ATOH	CA	LEU A 292	35.459	17.043	16.777	1.00	10.78	6
2405	ATOH	CG	LEU A 292	34.525	18.220	17.143	1.00	11.55	6
2406	ATOH	CG	LEU A 292	33.126	17.717	17.616	1.00	10.98	6
2407	ATOH	CD1	LEU A 292	32.406	18.847	18.358	1.00	10.98	6
2408	ATOH	CD2	LEU A 292	32.371	17.124	16.439	1.00	11.27	6
2409	ATOH	C	LEU A 292	36.713	17.628	16.088	1.00	11.19	6
2410	ATOH	O	LEU A 292	36.821	17.685	14.878	1.00	11.27	8
2411	ATOH	N	GLN A 293	37.674	18.093	16.832	1.00	11.50	7
2412	ATOH	CA	GLN A 293	38.899	18.619	16.322	1.00	12.28	6
2413	ATOH	CG	GLN A 293	39.632	19.090	17.572	1.00	15.35	6
2414	ATOH	CG	GLN A 293	40.644	20.159	17.294	1.00	20.28	6
2415	ATOH	CD	GLN A 293	42.018	19.550	17.111	1.00	23.63	6
2416	ATOH	CD1	GLN A 293	42.277	18.617	17.883	1.00	27.19	8
2417	ATOH	CD2	GLN A 293	42.755	20.086	16.154	1.00	25.26	7
2418	ATOH	C	GLN A 293	39.771	17.574	15.581	1.00	12.47	6
2419	ATOH	O	GLN A 293	40.424	17.827	14.578	1.00	12.05	8
2420	ATOH	N	ALA A 294	39.793	16.376	16.196	1.00	13.37	6
2421	ATOH	CA	ALA A 294	40.557	15.278	15.655	1.00	12.83	7
2422	ATOH	CB	ALA A 294	40.630	14.069	16.503	1.00	12.51	6
2423	ATOH	C	ALA A 294	39.920	14.904	14.299	1.00	13.89	6
2424	ATOH	O	ALA A 294	40.681	14.764	13.312	1.00	14.17	8
2425	ATOH	N	ALA A 295	38.580	14.804	14.185	1.00	13.85	7
2426	ATOH	CA	ALA A 295	37.963	14.486	12.906	1.00	13.85	6
2427	ATOH	CB	ALA A 295	36.447	14.351	12.963	1.00	11.81	6
2428	ATOH	C	ALA A 295	38.280	15.584	11.874	1.00	14.11	6
2429	ATOH	O	ALA A 295	38.474	15.301	10.678	1.00	14.15	8
2430	ATOH	N	SER A 296	38.311	16.845	12.322	1.00	14.00	7
2431	ATOH	CA	SER A 296	38.562	17.954	11.422	1.00	14.17	6
2432	ATOH	CB	SER A 296	38.176	19.248	12.167	1.00	10.42	6
2433	ATOH	CG	SER A 296	39.176	19.868	12.880	1.00	8.51	8
2434	ATOH	C	SER A 296	40.000	17.997	10.859	1.00	14.43	6
2435	ATOH	O	SER A 296	40.338	18.622	9.838	1.00	14.12	8
2436	ATOH	N	SER A 297	40.902	17.322	11.540	1.00	14.82	7
2437	ATOH	CA	SER A 297	42.305	17.287	11.269	1.00	15.50	6
2438	ATOH	CB	SER A 297	42.931	16.991	12.708	1.00	16.67	6

ATOM	2439	OG	SER A 297	42.921	18.303	13.176	1.00	20.24	8
ATOM	2440	C	SER A 297	42.921	16.146	10.508	1.00	15.90	6
ATOM	2441	O	SER A 297	44.076	16.216	10.160	1.00	15.87	8
ATOM	2442	N	GLN A 298	42.143	15.074	10.370	1.00	16.33	7
ATOM	2443	CA	GLN A 298	42.650	13.888	9.722	1.00	16.82	6
ATOM	2444	CB	GLN A 298	42.156	12.653	10.523	1.00	18.92	6
ATOM	2445	CG	GLN A 298	43.084	12.447	11.693	1.00	20.51	6
ATOM	2446	CD	GLN A 298	42.613	11.548	12.798	1.00	23.02	6
ATOM	2447	OE1	GLN A 298	42.174	10.410	12.588	1.00	24.09	8
ATOM	2448	HE2	GLN A 298	42.715	12.077	14.034	1.00	23.74	7
ATOM	2449	C	GLN A 298	42.319	13.823	8.245	1.00	17.02	6
ATOM	2450	O	GLN A 298	42.486	12.719	7.679	1.00	17.29	8
ATOM	2451	N	GLY A 299	41.907	14.913	7.631	1.00	16.90	7
ATOM	2452	CA	GLY A 299	41.595	15.001	6.223	1.00	16.90	6
ATOM	2453	C	GLY A 299	40.763	13.864	5.685	1.00	16.77	6
ATOM	2454	O	GLY A 299	40.942	13.480	4.523	1.00	17.33	8
ATOM	2455	N	GLY A 300	39.855	13.274	6.435	1.00	16.11	7
ATOM	2456	CA	GLY A 300	39.068	12.163	5.983	1.00	15.25	6
ATOM	2457	C	GLY A 300	39.483	10.868	6.650	1.00	14.82	6
ATOM	2458	O	GLY A 300	38.603	10.027	6.489	1.00	14.53	8
ATOM	2459	N	GLY A 301	40.574	10.532	7.302	1.00	14.47	7
ATOM	2460	CA	GLY A 301	40.815	9.227	7.860	1.00	14.37	6
ATOM	2461	C	GLY A 301	40.234	8.948	9.225	1.00	14.36	6
ATOM	2462	O	GLY A 301	40.318	7.830	9.696	1.00	14.17	8
ATOM	2463	N	TYR A 302	39.559	9.888	9.908	1.00	14.62	7
ATOM	2464	CA	TYR A 302	38.973	9.650	11.220	1.00	14.57	6
ATOM	2465	C	TYR A 302	38.419	10.956	11.845	1.00	14.59	6
ATOM	2466	CG	TYR A 302	37.750	10.869	13.198	1.00	14.61	6
ATOM	2467	CD1	TYR A 302	38.559	10.860	14.355	1.00	14.96	6
ATOM	2468	CE1	TYR A 302	37.990	10.754	15.630	1.00	14.98	6
ATOM	2469	CD2	TYR A 302	36.380	10.751	13.400	1.00	14.40	6
ATOM	2470	CE2	TYR A 302	35.820	10.629	14.663	1.00	14.56	6
ATOM	2471	CZ	TYR A 302	36.622	10.655	15.778	1.00	14.83	6
ATOM	2472	OH	TYR A 302	36.157	10.564	17.049	1.00	15.01	8
ATOM	2473	C	TYR A 302	37.831	8.643	11.151	1.00	14.74	6
ATOM	2474	O	TYR A 302	37.073	8.682	10.170	1.00	14.62	8
ATOM	2475	N	ASP A 303	37.515	7.744	12.058	1.00	14.71	7
ATOM	2476	CA	ASP A 303	36.350	6.873	11.910	1.00	14.90	6
ATOM	2477	CB	ASP A 303	36.617	5.550	12.620	1.00	16.31	6
ATOM	2478	CG	ASP A 303	35.526	4.517	12.403	1.00	17.88	6
ATOM	2479	CD1	ASP A 303	34.383	4.796	12.005	1.00	17.07	8
ATOM	2480	CD2	ASP A 303	35.893	3.348	12.637	1.00	19.55	8
ATOM	2481	C	ASP A 303	35.165	7.627	12.500	1.00	14.85	8
ATOM	2482	O	ASP A 303	35.013	7.729	13.714	1.00	14.59	8
ATOM	2483	N	HET A 304	34.315	8.199	11.658	1.00	14.94	7
ATOM	2484	CA	HET A 304	33.151	8.973	12.057	1.00	15.29	6
ATOM	2485	CB	HET A 304	32.440	9.630	10.862	1.00	14.35	6
ATOM	2486	CG	HET A 304	33.307	10.718	10.201	1.00	13.91	6
ATOM	2487	CD	HET A 304	33.391	12.309	11.028	1.00	14.76	16
ATOM	2488	CE	HET A 304	31.941	13.156	10.378	1.00	11.94	6
ATOM	2489	C	HET A 304	32.161	8.195	12.917	1.00	15.60	6
ATOM	2490	O	HET A 304	31.322	8.846	13.569	1.00	15.54	8
ATOM	2491	N	ARG A 305	32.251	6.872	13.019	1.00	15.77	7
ATOM	2492	CA	ARG A 305	31.372	6.123	13.883	1.00	16.15	6
ATOM	2493	CB	ARG A 305	31.398	4.601	13.558	1.00	17.94	6
ATOM	2494	CG	ARG A 305	30.663	4.270	12.266	1.00	20.53	6
ATOM	2495	CD	ARG A 305	30.984	3.018	11.512	1.00	21.54	6
ATOM	2496	CE	ARG A 305	32.390	2.813	11.326	1.00	23.87	7
ATOM	2497	CZ	ARG A 305	32.917	1.717	10.819	1.00	26.93	6
ATOM	2498	HH1	ARG A 305	32.145	0.716	10.412	1.00	29.01	7
ATOM	2499	HH2	ARG A 305	34.239	1.652	10.753	1.00	28.19	7
ATOM	2500	C	ARG A 305	31.768	6.318	15.354	1.00	16.33	6
ATOM	2501	O	ARG A 305	30.997	5.924	16.218	1.00	16.15	8
ATOM	2502	N	LYS A 306	32.942	6.837	15.661	1.00	16.51	7
ATOM	2503	CA	LYS A 306	33.424	7.006	17.011	1.00	17.04	6
ATOM	2504	CB	LYS A 306	34.945	6.643	16.903	1.00	19.89	6
ATOM	2505	CG	LYS A 306	35.043	5.174	16.504	1.00	25.08	6
ATOM	2506	CD	LYS A 306	36.487	4.726	16.705	1.00	30.20	6
ATOM	2507	CE	LYS A 306	36.968	3.663	15.712	1.00	32.87	6
ATOM	2508	NZ	LYS A 306	37.911	2.695	16.442	1.00	35.11	7
ATOM	2509	O	LYS A 306	33.356	8.375	17.653	1.00	17.07	6
ATOM	2510	O	LYS A 306	33.967	8.639	18.692	1.00	16.98	8
ATOM	2511	N	LEU A 307	32.639	9.313	17.026	1.00	17.11	7
ATOM	2512	CA	LEU A 307	32.539	10.700	17.444	1.00	17.21	6
ATOM	2513	CB	LEU A 307	31.608	11.509	16.526	1.00	18.35	6
ATOM	2514	CG	LEU A 307	32.192	12.263	15.348	1.00	20.88	6
ATOM	2515	CD1	LEU A 307	31.055	12.963	14.582	1.00	21.03	6
ATOM	2516	CD2	LEU A 307	33.273	13.283	15.684	1.00	20.35	6
ATOM	2517	C	LEU A 307	32.084	10.826	18.890	1.00	17.01	6
ATOM	2518	O	LEU A 307	32.553	11.677	19.605	1.00	17.09	8
ATOM	2519	N	LEU A 308	31.179	9.970	19.331	1.00	16.89	7
ATOM	2520	CA	LEU A 308	30.629	9.973	20.670	1.00	16.75	6
ATOM	2521	CB	LEU A 308	29.153	9.440	20.589	1.00	17.24	6
ATOM	2522	CG	LEU A 308	28.116	10.476	20.136	1.00	19.15	6
ATOM	2523	CD1	LEU A 308	26.740	9.862	19.977	1.00	18.81	6
ATOM	2524	CD2	LEU A 308	28.015	11.685	21.063	1.00	19.79	6
ATOM	2525	C	LEU A 308	31.420	9.200	21.720	1.00	16.38	6
ATOM	2526	O	LEU A 308	31.137	9.327	22.922	1.00	16.30	8
ATOM	2527	N	ASN A 309	32.381	8.386	21.344	1.00	16.16	7
ATOM	2528	CA	ASN A 309	33.203	7.595	22.228	1.00	15.89	6
ATOM	2529	CB	ASN A 309	34.349	6.886	21.492	1.00	21.07	6
ATOM	2530	CG	ASN A 309	33.880	5.720	20.660	1.00	26.35	6
ATOM	2531	CD1	ASN A 309	34.746	5.049	20.024	1.00	29.82	8
ATOM	2532	CD2	ASN A 309	32.579	5.435	20.588	1.00	27.51	7
ATOM	2533	C	ASN A 309	33.938	8.456	23.265	1.00	15.16	6
ATOM	2534	O	ASN A 309	34.623	9.384	22.831	1.00	15.00	8
ATOM	2535	N	GLY A 310	33.777	8.102	24.545	1.00	14.32	7
ATOM	2536	CA	GLY A 310	34.447	8.836	25.603	1.00	13.49	6
ATOM	2537	C	GLY A 310	33.944	10.232	25.938	1.00	12.69	6
ATOM	2538	O	GLY A 310	34.667	10.890	26.657	1.00	12.41	8
ATOM	2539	N	THR A 311	32.784	10.615	25.413	1.00	12.19	7
ATOM	2540	CA	THR A 311	32.222	11.929	25.676	1.00	11.65	6
ATOM	2541	CB	THR A 311	31.462	12.519	24.452	1.00	10.26	6
ATOM	2542	CG	THR A 311	30.315	11.692	24.240	1.00	10.86	8
ATOM	2543	CG2	THR A 311	32.307	12.571	23.191	1.00	8.42	6
ATOM	2544	C	THR A 311	31.284	11.908	26.895	1.00	11.36	6

2545	ATOH	2545	O	THR A 311	30.667	10.902	27.258	1.00	11.29	8
2546	ATOH	2546	N	VAL A 312	31.198	13.075	27.545	1.00	11.20	7
2547	ATOH	2547	CA	VAL A 312	30.313	13.282	28.693	1.00	11.29	6
2548	ATOH	2548	CB	VAL A 312	30.567	14.637	29.407	1.00	12.62	6
2549	ATOH	2549	CG1	VAL A 312	29.620	14.906	30.597	1.00	13.45	6
2550	ATOH	2550	CG2	VAL A 312	31.995	14.730	29.912	1.00	10.56	6
2551	ATOH	2551	C	VAL A 312	28.874	13.189	28.191	1.00	11.23	6
2552	ATOH	2552	O	VAL A 312	28.053	12.526	28.793	1.00	11.01	8
2553	ATOH	2553	N	VAL A 313	28.533	13.825	27.061	1.00	11.42	7
2554	ATOH	2554	CA	VAL A 313	27.208	13.790	26.498	1.00	11.94	6
2555	ATOH	2555	CB	VAL A 313	27.107	14.723	25.266	1.00	12.88	6
2556	ATOH	2556	CG1	VAL A 313	27.604	14.175	23.942	1.00	13.11	6
2557	ATOH	2557	CG2	VAL A 313	25.627	15.102	25.100	1.00	14.06	6
2558	ATOH	2558	O	VAL A 313	26.655	12.380	26.219	1.00	12.21	6
2559	ATOH	2559	N	SER A 314	25.434	12.216	26.319	1.00	11.69	8
2560	ATOH	2560	H	SER A 314	27.418	11.313	25.971	1.00	12.83	7
2561	ATOH	2561	CA	SER A 314	26.878	9.987	25.750	1.00	13.63	6
2562	ATOH	2562	CB	SER A 314	27.801	9.054	24.922	1.00	13.56	6
2563	ATOH	2563	OG	SER A 314	29.056	9.048	25.641	1.00	15.90	8
2564	ATOH	2564	C	SER A 314	26.572	9.345	27.111	1.00	14.04	6
2565	ATOH	2565	O	SER A 314	25.730	8.445	27.105	1.00	14.28	8
2566	ATOH	2566	N	LVS A 315	27.168	9.725	28.254	1.00	14.23	7
2567	ATOH	2567	CA	LVS A 315	26.823	9.081	29.513	1.00	14.22	6
2568	ATOH	2568	CB	LVS A 315	27.928	8.797	30.491	1.00	19.81	6
2569	ATOH	2569	CG	LVS A 315	30.321	8.495	30.319	1.00	26.75	6
2570	ATOH	2570	CD	LVS A 315	30.321	9.661	30.402	1.00	32.49	6
2571	ATOH	2571	CE	LVS A 315	30.714	10.114	31.825	1.00	35.30	6
2572	ATOH	2572	H2	LVS A 315	31.599	9.199	32.634	1.00	35.57	7
2573	ATOH	2573	C	LVS A 315	25.884	9.951	30.379	1.00	13.74	6
2574	ATOH	2574	O	LVS A 315	24.969	9.435	31.020	1.00	13.60	8
2575	ATOH	2575	N	HIS A 316	26.108	11.257	30.397	1.00	13.12	7
2576	ATOH	2576	CA	HIS A 316	25.314	12.197	31.179	1.00	13.02	6
2577	ATOH	2577	CB	HIS A 316	26.202	12.791	32.327	1.00	12.69	6
2578	ATOH	2578	CG	HIS A 316	26.550	11.718	33.313	1.00	12.94	6
2579	ATOH	2579	CD2	HIS A 316	25.796	11.024	34.166	1.00	13.25	6
2580	ATOH	2580	HD1	HIS A 316	27.835	11.194	33.424	1.00	15.42	7
2581	ATOH	2581	CE1	HIS A 316	27.850	10.206	34.317	1.00	14.97	6
2582	ATOH	2582	HE2	HIS A 316	26.617	10.106	34.822	1.00	15.47	7
2583	ATOH	2583	C	HIS A 316	24.809	13.360	30.325	1.00	12.64	6
2584	ATOH	2584	O	HIS A 316	25.304	14.479	30.471	1.00	12.29	8
2585	ATOH	2585	N	PRO A 317	23.868	13.075	29.435	1.00	12.52	7
2586	ATOH	2586	CD	PRO A 317	23.256	11.760	29.268	1.00	12.43	6
2587	ATOH	2587	CA	PRO A 317	23.311	14.040	28.519	1.00	12.50	6
2588	ATOH	2588	CB	PRO A 317	22.280	13.268	27.640	1.00	12.54	6
2589	ATOH	2589	CG	PRO A 317	21.996	12.051	28.524	1.00	12.55	6
2590	ATOH	2590	C	PRO A 317	22.669	15.253	29.133	1.00	12.59	6
2591	ATOH	2591	O	PRO A 317	22.750	16.349	28.542	1.00	12.88	8
2592	ATOH	2592	N	LEU A 318	21.370	16.286	30.956	1.00	12.38	6
2593	ATOH	2593	CA	LEU A 318	22.033	15.168	30.285	1.00	12.44	7
2594	ATOH	2594	CB	LEU A 318	20.278	15.805	31.970	1.00	13.77	6
2595	ATOH	2595	CG	LEU A 318	19.256	14.834	31.334	1.00	15.85	6
2596	ATOH	2596	CD1	LEU A 318	18.250	14.143	32.241	1.00	15.19	6
2597	ATOH	2597	CD2	LEU A 318	18.520	15.629	30.254	1.00	17.19	6
2598	ATOH	2598	O	LEU A 318	22.338	17.175	31.741	1.00	11.91	6
2599	ATOH	2599	O	LEU A 318	21.929	18.174	32.286	1.00	11.51	8
2600	ATOH	2600	N	LVS A 319	23.602	16.757	31.836	1.00	11.53	7
2601	ATOH	2601	CA	LVS A 319	24.559	17.559	32.591	1.00	11.24	6
2602	ATOH	2602	CB	LVS A 319	25.135	16.758	33.794	1.00	12.25	6
2603	ATOH	2603	CG	LVS A 319	24.001	16.369	34.812	1.00	12.23	6
2604	ATOH	2604	CD	LVS A 319	23.655	17.705	35.470	1.00	13.91	6
2605	ATOH	2605	CE	LVS A 319	22.335	17.774	36.181	1.00	15.19	6
2606	ATOH	2606	H2	LVS A 319	22.278	18.963	37.119	1.00	14.09	7
2607	ATOH	2607	C	LVS A 319	25.652	18.008	31.640	1.00	10.89	6
2608	ATOH	2608	O	LVS A 319	26.717	18.376	32.153	1.00	11.10	8
2609	ATOH	2609	N	SER A 320	25.462	17.969	30.320	1.00	10.24	7
2610	ATOH	2610	CA	SER A 320	26.564	18.409	29.483	1.00	9.74	6
2611	ATOH	2611	CB	SER A 320	26.825	17.443	28.311	1.00	11.44	6
2612	ATOH	2612	OG	SER A 320	26.960	16.158	28.752	1.00	15.00	8
2613	ATOH	2613	C	SER A 320	26.322	19.681	28.692	1.00	9.08	6
2614	ATOH	2614	O	SER A 320	25.215	19.672	28.144	1.00	9.21	8
2615	ATOH	2615	N	VAL A 321	27.294	20.549	28.581	1.00	8.35	7
2616	ATOH	2616	CA	VAL A 321	27.166	21.744	27.760	1.00	7.87	6
2617	ATOH	2617	CB	VAL A 321	27.455	23.085	28.447	1.00	6.55	6
2618	ATOH	2618	CG1	VAL A 321	27.468	24.283	27.473	1.00	5.70	6
2619	ATOH	2619	CG2	VAL A 321	26.352	23.381	29.489	1.00	6.25	6
2620	ATOH	2620	C	VAL A 321	28.079	21.422	26.585	1.00	7.79	6
2621	ATOH	2621	O	VAL A 321	29.282	21.146	26.791	1.00	8.06	8
2622	ATOH	2622	N	THR A 322	27.497	21.399	25.396	1.00	7.46	7
2623	ATOH	2623	CA	THR A 322	28.302	21.038	24.183	1.00	7.12	6
2624	ATOH	2624	CB	THR A 322	27.504	20.146	23.199	1.00	5.50	6
2625	ATOH	2625	OG1	THR A 322	26.184	20.559	22.923	1.00	5.00	8
2626	ATOH	2626	CG2	THR A 322	27.279	18.718	23.807	1.00	6.18	6
2627	ATOH	2627	C	THR A 322	28.877	22.262	23.492	1.00	7.07	6
2628	ATOH	2628	O	THR A 322	28.206	23.319	23.510	1.00	7.34	8
2629	ATOH	2629	N	PIE A 323	30.076	22.181	22.907	1.00	6.79	7
2630	ATOH	2630	CA	PIE A 323	30.734	23.301	22.257	1.00	6.58	6
2631	ATOH	2631	CB	PIE A 323	31.435	24.192	23.312	1.00	5.72	6
2632	ATOH	2632	CG	PIE A 323	32.752	23.783	23.849	1.00	5.21	6
2633	ATOH	2633	CD1	PIE A 323	33.918	24.279	23.270	1.00	6.61	6
2634	ATOH	2634	CD2	PIE A 323	32.864	22.861	24.884	1.00	6.77	6
2635	ATOH	2635	CE1	PIE A 323	35.167	23.880	23.764	1.00	7.34	6
2636	ATOH	2636	CE2	PIE A 323	34.105	22.368	25.363	1.00	6.08	6
2637	ATOH	2637	C	PIE A 323	35.238	22.944	24.795	1.00	6.00	6
2638	ATOH	2638	O	PIE A 323	31.727	22.855	21.184	1.00	6.75	6
2639	ATOH	2639	N	PIE A 323	32.313	21.743	21.207	1.00	6.74	8
2640	ATOH	2640	CA	VAL A 324	31.917	23.744	20.208	1.00	6.84	7
2641	ATOH	2641	CB	VAL A 324	32.846	23.539	19.087	1.00	6.92	6
2642	ATOH	2642	CB	VAL A 324	33.175	23.923	16.595	1.00	5.00	6
2643	ATOH	2643	CG1	VAL A 324	30.945	23.335	17.428	1.00	5.00	6
2644	ATOH	2644	CG2	VAL A 324	34.230	24.137	19.434	1.00	7.23	6
2645	ATOH	2645	C	VAL A 324	35.247	23.410	19.508	1.00	6.91	8
2646	ATOH	2646	O	VAL A 324	34.276	25.479	19.678	1.00	7.39	7
2647	ATOH	2647	N	ASP A 325	35.469	26.189	20.078	1.00	7.78	6
2648	ATOH	2648	CA	ASP A 325	36.180	26.898	18.918	1.00	8.62	6
2649	ATOH	2649	CB	ASP A 325	37.157	25.954	18.192	1.00	8.81	6
2650	ATOH	2650	CG	ASP A 325						

2651	001 ASP A 325	38.076	25.409	18.839	1.00	7.66	8	7
2652	002 ASP A 325	37.027	25.682	16.964	1.00	9.34	8	6
2653	C ASP A 325	35.117	27.261	21.116	1.00	8.18	6	6
2654	O ASP A 325	33.960	27.635	21.254	1.00	8.16	8	8
2655	N ASH A 326	36.108	27.788	21.826	1.00	8.35	7	7
2656	CA ASH A 326	35.925	28.845	22.813	1.00	8.28	6	6
2657	CB ASH A 326	35.487	28.329	24.160	1.00	9.54	6	6
2658	CG ASH A 326	36.502	27.485	24.902	1.00	11.91	6	6
2659	001 ASH A 326	37.701	27.415	24.622	1.00	12.52	8	6
2660	002 ASH A 326	36.121	26.782	25.965	1.00	11.95	7	6
2661	C ASH A 326	37.212	29.685	22.871	1.00	8.44	6	7
2662	O ASH A 326	38.140	29.601	22.053	1.00	7.98	8	6
2663	N H1S A 327	37.266	30.626	23.836	1.00	8.65	7	6
2664	CA H1S A 327	38.367	31.562	23.994	1.00	9.17	6	8
2665	CB H1S A 327	37.976	32.718	24.999	1.00	8.48	6	6
2666	CG H1S A 327	37.800	32.154	26.392	1.00	7.81	6	6
2667	001 H1S A 327	38.481	32.357	27.535	1.00	7.34	6	8
2668	002 H1S A 327	36.785	31.222	26.672	1.00	8.46	7	6
2669	CE1 H1S A 327	36.886	30.856	27.951	1.00	7.98	6	6
2670	HE2 H1S A 327	37.883	31.538	28.493	1.00	8.30	7	8
2671	C H1S A 327	39.664	30.866	24.404	1.00	9.58	6	7
2672	O H1S A 327	40.718	31.444	24.169	1.00	9.63	8	6
2673	N ASP A 328	39.645	29.653	24.928	1.00	10.01	7	6
2674	CA ASP A 328	40.783	28.869	25.312	1.00	10.53	6	6
2675	CB ASP A 328	40.422	27.735	26.312	1.00	14.56	6	6
2676	CG ASP A 328	39.676	27.936	27.629	1.00	18.50	6	6
2677	001 ASP A 328	40.162	28.843	28.385	1.00	17.22	8	6
2678	002 ASP A 328	38.615	27.265	28.055	1.00	18.97	8	6
2679	C ASP A 328	41.385	28.188	24.074	1.00	10.65	6	6
2680	O ASP A 328	42.607	28.041	23.933	1.00	10.58	8	6
2681	N H1R A 329	40.518	27.688	23.167	1.00	10.47	7	6
2682	CA H1R A 329	40.946	26.880	22.028	1.00	10.37	6	6
2683	CB H1R A 329	39.933	25.709	21.777	1.00	10.26	6	6
2684	CG H1R A 329	38.709	26.293	21.286	1.00	9.63	8	6
2685	001 H1R A 329	39.596	24.873	23.020	1.00	9.29	6	6
2686	002 H1R A 329	41.142	27.596	20.702	1.00	10.36	6	6
2687	C H1R A 329	41.563	26.999	19.704	1.00	9.94	8	6
2688	N GLN A 330	40.827	28.878	20.679	1.00	10.77	7	6
2689	CA GLN A 330	40.985	29.688	19.441	1.00	11.30	6	6
2690	CG GLN A 330	40.182	30.988	19.518	1.00	9.13	6	6
2691	C GLN A 330	40.769	31.987	20.543	1.00	8.40	6	6
2692	001 GLN A 330	40.003	33.322	20.559	1.00	8.44	6	6
2693	002 GLN A 330	39.089	33.499	21.393	1.00	7.21	8	6
2694	HE2 GLN A 330	40.432	34.237	19.660	1.00	7.16	7	6
2695	C GLN A 330	42.486	29.890	19.211	1.00	11.99	6	6
2696	O GLN A 330	43.345	29.690	20.092	1.00	11.70	8	6
2697	N PRO A 331	42.793	30.208	17.963	1.00	12.85	7	6
2698	CA PRO A 331	41.806	30.403	16.873	1.00	12.95	6	6
2699	CG PRO A 331	44.119	30.424	17.447	1.00	13.52	6	6
2700	CB PRO A 331	43.974	30.918	15.966	1.00	13.53	6	6
2701	CG PRO A 331	42.608	30.336	15.583	1.00	13.10	6	6
2702	C PRO A 331	44.899	31.372	18.320	1.00	14.55	6	6
2703	O PRO A 331	44.496	32.463	18.767	1.00	14.46	8	6
2704	N GLY A 332	46.122	30.893	18.593	1.00	15.77	7	6
2705	CA GLY A 332	47.087	31.624	19.404	1.00	17.06	6	6
2706	C GLY A 332	46.881	31.463	20.896	1.00	18.22	6	6
2707	O GLY A 332	47.755	31.915	21.633	1.00	18.26	8	6
2708	N GLN A 333	45.817	30.862	21.429	1.00	19.06	7	6
2709	CA GLN A 333	45.678	30.778	22.875	1.00	19.88	6	6
2710	CG GLN A 333	44.181	30.838	23.241	1.00	19.70	6	6
2711	CD GLN A 333	43.711	32.283	23.072	1.00	20.78	6	6
2712	OE1 GLN A 333	44.572	33.254	23.876	1.00	23.47	6	6
2713	HE2 GLN A 333	45.181	34.191	23.315	1.00	26.12	8	6
2714	C GLN A 333	44.705	33.056	25.175	1.00	22.30	7	6
2715	O GLN A 333	46.462	29.622	23.446	1.00	20.87	6	6
2716	N SER A 334	47.167	28.850	22.773	1.00	20.84	8	6
2717	CA SER A 334	46.339	29.555	24.795	1.00	21.65	7	6
2718	CG SER A 334	47.083	28.519	25.552	1.00	22.42	6	6
2719	CD SER A 334	46.792	28.705	27.067	1.00	26.55	6	6
2720	OE1 SER A 334	45.405	29.089	27.235	1.00	30.85	8	6
2721	C SER A 334	46.790	27.074	25.194	1.00	22.23	6	6
2722	O SER A 334	47.687	26.293	24.929	1.00	22.55	8	6
2723	N LEU A 335	45.506	26.728	25.170	1.00	21.74	7	6
2724	CA LEU A 335	44.958	25.411	24.863	1.00	20.75	6	6
2725	CG LEU A 335	43.814	25.183	25.883	1.00	22.84	6	6
2726	CD LEU A 335	44.252	25.266	27.365	1.00	23.70	6	6
2727	OE1 LEU A 335	43.065	25.292	28.305	1.00	23.07	6	6
2728	C LEU A 335	45.184	24.089	27.673	1.00	24.51	6	6
2729	O LEU A 335	44.460	25.313	23.427	1.00	19.68	6	6
2730	N GLU A 336	43.491	24.609	23.136	1.00	19.77	8	6
2731	CA GLU A 336	45.111	26.053	22.536	1.00	18.47	7	6
2732	CG GLU A 336	44.766	26.089	21.149	1.00	17.45	6	6
2733	CD GLU A 336	45.908	26.773	20.387	1.00	19.49	6	6
2734	OE1 GLU A 336	45.655	26.544	18.905	1.00	22.99	6	6
2735	C GLU A 336	46.508	27.440	18.036	1.00	26.38	6	6
2736	O GLU A 336	47.378	28.166	18.504	1.00	26.94	8	6
2737	N SER A 337	46.276	27.487	16.805	1.00	28.18	8	6
2738	CA SER A 337	44.504	24.698	20.571	1.00	16.40	6	6
2739	CG SER A 337	45.349	23.802	20.647	1.00	16.09	8	6
2740	CD SER A 337	43.338	24.527	19.954	1.00	15.33	7	6
2741	OE1 SER A 337	43.005	23.217	19.393	1.00	14.23	6	6
2742	C SER A 337	42.891	22.175	20.487	1.00	13.48	6	6
2743	O SER A 337	41.855	22.515	21.439	1.00	13.96	8	6
2744	N THR A 338	41.679	23.436	18.645	1.00	13.82	6	6
2745	CA THR A 338	40.615	22.864	18.896	1.00	13.37	7	6
2746	CG THR A 338	41.878	24.333	17.679	1.00	13.53	8	6
2747	CD THR A 338	40.800	24.801	16.837	1.00	13.46	6	6
2748	OE1 THR A 338	41.340	26.036	16.033	1.00	13.02	6	6
2749	C THR A 338	40.259	26.794	15.338	1.00	12.29	6	6
2750	O THR A 338	40.216	23.770	15.877	1.00	13.20	6	6
2751	N VAL A 339	40.980	23.008	15.281	1.00	13.26	8	6
2752	CA VAL A 339	38.905	23.766	15.743	1.00	12.73	7	6
2753	CG VAL A 339	38.270	22.857	14.783	1.00	12.66	6	6
2754	CD VAL A 339	36.803	22.594	15.154	1.00	11.55	6	6
2755	OE1 VAL A 339	36.030	21.874	14.057	1.00	9.87	6	6

ATOM	2757	CG2	VAL	A	339	36.745	21.811	16.483	1.00	9.86	6	6
ATOM	2758	C	VAL	A	339	38.513	23.484	13.385	1.00	12.57	6	6
ATOM	2759	O	VAL	A	339	38.271	24.688	13.279	1.00	12.26	8	7
ATOM	2760	N	GLN	A	340	39.016	22.686	12.404	1.00	12.55	7	8
ATOM	2761	CA	GLN	A	340	39.280	23.302	11.088	1.00	12.55	6	6
ATOM	2762	CB	GLN	A	340	39.975	22.357	10.097	1.00	11.11	6	6
ATOM	2763	CG	GLN	A	340	41.372	21.974	10.559	1.00	11.55	6	6
ATOM	2764	CD	GLN	A	340	42.073	21.105	9.513	1.00	14.34	6	6
ATOM	2765	OE1	GLN	A	340	41.594	20.802	8.384	1.00	15.11	8	8
ATOM	2766	HE2	GLN	A	340	43.272	20.743	9.959	1.00	12.61	7	7
ATOM	2767	C	GLN	A	340	38.009	23.900	10.468	1.00	12.34	6	6
ATOM	2768	O	GLN	A	340	36.930	23.331	10.565	1.00	12.28	8	8
ATOM	2769	N	THR	A	341	38.147	25.042	9.779	1.00	12.25	7	7
ATOM	2770	CA	THR	A	341	37.024	25.755	9.200	1.00	12.38	6	6
ATOM	2771	CB	THR	A	341	37.514	26.993	8.393	1.00	15.06	6	6
ATOM	2772	CG1	THR	A	341	38.100	27.874	9.353	1.00	16.92	8	8
ATOM	2773	CG2	THR	A	341	36.347	27.684	7.716	1.00	14.77	6	6
ATOM	2774	C	THR	A	341	36.124	24.916	8.332	1.00	12.08	6	6
ATOM	2775	O	THR	A	341	34.910	25.018	8.411	1.00	12.16	8	8
ATOM	2776	N	TRP	A	342	36.698	24.095	7.465	1.00	11.85	7	7
ATOM	2777	CA	TRP	A	342	35.902	23.225	6.585	1.00	11.19	6	6
ATOM	2778	CB	TRP	A	342	36.871	22.438	6.373	1.00	10.89	6	6
ATOM	2779	CG	TRP	A	342	37.568	21.288	6.392	1.00	9.86	6	6
ATOM	2780	CD2	TRP	A	342	37.073	19.949	6.491	1.00	9.37	6	6
ATOM	2781	CE2	TRP	A	342	37.988	19.219	7.276	1.00	9.97	6	6
ATOM	2782	CE3	TRP	A	342	35.916	19.290	5.991	1.00	10.12	6	6
ATOM	2783	CD1	TRP	A	342	38.756	21.330	7.062	1.00	10.06	6	6
ATOM	2784	HE1	TRP	A	342	39.027	20.080	7.592	1.00	11.11	7	7
ATOM	2785	C22	TRP	A	342	37.809	17.853	7.527	1.00	10.50	6	6
ATOM	2786	C23	TRP	A	342	35.700	17.950	6.293	1.00	9.23	6	6
ATOM	2787	CI12	TRP	A	342	36.654	17.222	7.050	1.00	10.34	6	6
ATOM	2788	C	TRP	A	342	34.968	22.340	7.391	1.00	10.76	6	6
ATOM	2789	O	TRP	A	342	33.837	22.038	6.990	1.00	10.60	8	8
ATOM	2790	N	PIE	A	343	35.375	21.846	8.577	1.00	10.45	7	7
ATOM	2791	CA	PIE	A	343	34.544	20.979	9.389	1.00	9.81	6	6
ATOM	2792	CB	PIE	A	343	35.520	20.088	10.193	1.00	10.59	6	6
ATOM	2793	CG	PIE	A	343	34.841	18.880	10.796	1.00	9.94	6	6
ATOM	2794	CD1	PIE	A	343	34.561	17.786	9.989	1.00	9.97	6	6
ATOM	2795	CD2	PIE	A	343	34.466	18.875	12.117	1.00	9.30	6	6
ATOM	2796	CE1	PIE	A	343	33.947	16.653	10.504	1.00	9.66	6	6
ATOM	2797	CE2	PIE	A	343	33.842	17.747	12.659	1.00	10.16	6	6
ATOM	2798	CZ	PIE	A	343	33.592	16.637	11.845	1.00	10.55	6	6
ATOM	2799	C	PIE	A	343	33.621	21.720	10.332	1.00	9.65	6	6
ATOM	2800	O	PIE	A	343	32.649	21.140	10.826	1.00	9.50	8	8
ATOM	2801	N	LYS	A	344	33.897	23.010	10.569	1.00	9.52	7	7
ATOM	2802	CA	LYS	A	344	33.084	23.775	11.536	1.00	9.73	6	6
ATOM	2803	CB	LYS	A	344	33.689	25.209	11.614	1.00	11.03	6	6
ATOM	2804	CG	LYS	A	344	33.193	25.978	12.846	1.00	11.47	6	6
ATOM	2805	CD	LYS	A	344	34.235	26.954	13.366	1.00	10.60	6	6
ATOM	2806	CE	LYS	A	344	35.068	26.281	14.470	1.00	9.19	6	6
ATOM	2807	HZ	LYS	A	344	36.098	27.262	14.962	1.00	7.52	7	7
ATOM	2808	C	LYS	A	344	31.573	23.696	11.384	1.00	9.62	6	6
ATOM	2809	O	LYS	A	344	30.838	23.428	12.371	1.00	9.63	8	8
ATOM	2810	H	PRO	A	345	30.989	23.886	10.213	1.00	9.37	7	7
ATOM	2811	CD	PRO	A	345	31.697	24.236	8.991	1.00	9.33	6	6
ATOM	2812	CA	PRO	A	345	29.559	23.779	10.018	1.00	9.01	6	6
ATOM	2813	CB	PRO	A	345	29.285	24.245	8.592	1.00	9.17	6	6
ATOM	2814	CG	PRO	A	345	30.576	25.000	8.288	1.00	9.42	6	6
ATOM	2815	C	PRO	A	345	29.077	22.331	10.309	1.00	8.68	6	6
ATOM	2816	O	PRO	A	345	27.992	22.162	10.862	1.00	8.28	8	8
ATOM	2817	N	LEU	A	346	29.863	21.274	9.998	1.00	8.29	7	7
ATOM	2818	CA	LEU	A	346	29.491	19.890	10.274	1.00	7.82	6	6
ATOM	2819	CB	LEU	A	346	30.443	18.876	9.664	1.00	7.71	6	6
ATOM	2820	CG	LEU	A	346	30.608	18.730	8.147	1.00	9.48	6	6
ATOM	2821	CD1	LEU	A	346	30.910	20.053	7.472	1.00	6.38	6	6
ATOM	2822	CD2	LEU	A	346	31.710	17.710	7.794	1.00	7.94	6	6
ATOM	2823	C	LEU	A	346	29.426	19.714	11.796	1.00	7.55	6	6
ATOM	2824	O	LEU	A	346	28.510	19.084	12.262	1.00	7.43	8	8
ATOM	2825	N	ALA	A	347	30.320	20.297	12.583	1.00	7.30	7	7
ATOM	2826	CA	ALA	A	347	30.425	20.274	14.019	1.00	7.11	6	6
ATOM	2827	CB	ALA	A	347	31.760	20.902	14.501	1.00	7.21	6	6
ATOM	2828	C	ALA	A	347	29.264	21.031	14.671	1.00	7.06	6	6
ATOM	2829	O	ALA	A	347	28.712	20.558	15.670	1.00	7.03	8	8
ATOM	2830	N	TYR	A	348	28.827	22.160	14.103	1.00	7.17	7	7
ATOM	2831	CA	TYR	A	348	27.673	22.854	14.693	1.00	7.17	6	6
ATOM	2832	CB	TYR	A	348	27.650	24.299	14.175	1.00	7.45	6	6
ATOM	2833	CG	TYR	A	348	28.510	25.236	15.008	1.00	7.77	6	6
ATOM	2834	CD1	TYR	A	348	29.718	25.772	14.609	1.00	7.85	6	6
ATOM	2835	CE1	TYR	A	348	30.416	26.670	15.415	1.00	7.87	6	6
ATOM	2836	CD2	TYR	A	348	28.035	25.569	16.285	1.00	7.82	6	6
ATOM	2837	CE2	TYR	A	348	28.731	26.430	17.105	1.00	7.89	6	6
ATOM	2838	CZ	TYR	A	348	29.917	26.984	16.682	1.00	7.94	6	6
ATOM	2839	OH	TYR	A	348	30.609	27.789	17.576	1.00	7.87	8	8
ATOM	2840	C	TYR	A	348	26.404	22.081	14.387	1.00	7.12	6	6
ATOM	2841	O	TYR	A	348	25.461	22.029	15.193	1.00	7.05	8	8
ATOM	2842	N	ALA	A	349	26.328	21.385	13.223	1.00	6.87	7	7
ATOM	2843	CA	ALA	A	349	25.127	20.607	12.939	1.00	6.67	6	6
ATOM	2844	CB	ALA	A	349	25.131	20.070	11.515	1.00	6.51	6	6
ATOM	2845	C	ALA	A	349	25.054	19.497	13.978	1.00	6.62	6	6
ATOM	2846	O	ALA	A	349	23.995	19.114	14.487	1.00	6.43	8	8
ATOM	2847	N	PIE	A	350	26.237	18.899	14.250	1.00	6.67	7	7
ATOM	2848	CA	PIE	A	350	26.268	17.814	15.220	1.00	6.81	6	6
ATOM	2849	CB	PIE	A	350	27.701	17.250	15.304	1.00	6.91	6	6
ATOM	2850	CG	PIE	A	350	27.746	15.996	16.137	1.00	9.15	6	6
ATOM	2851	CD1	PIE	A	350	27.494	14.763	15.559	1.00	8.95	6	6
ATOM	2852	CD2	PIE	A	350	28.009	16.069	17.510	1.00	11.23	6	6
ATOM	2853	CE1	PIE	A	350	27.551	13.618	16.317	1.00	10.89	6	6
ATOM	2854	CE2	PIE	A	350	28.044	14.894	18.273	1.00	11.66	6	6
ATOM	2855	CZ	PIE	A	350	27.847	13.657	17.687	1.00	10.74	6	6
ATOM	2856	C	PIE	A	350	25.768	18.242	16.605	1.00	6.90	6	6
ATOM	2857	O	PIE	A	350	24.978	17.547	17.275	1.00	6.86	8	8
ATOM	2858	N	ILE	A	351	26.217	19.408	17.102	1.00	7.14	7	7
ATOM	2859	CA	ILE	A	351	25.736	19.797	18.437	1.00	7.28	6	6
ATOM	2860	CB	ILE	A	351	26.767	20.663	19.194	1.00	6.43	6	6
ATOM	2861	CG2	ILE	A	351	28.084	19.924	19.275	1.00	6.52	6	6
ATOM	2862	CG1	ILE	A	351	26.943	22.024	18.556	1.00	6.43	6	6

ATOM	2863	CD1	ILE	A	351	27.589	22.986	19.575	1.00	5.33	6	ATOM	2916	CE1	TYR	A	358	21.449	26.080	26.747	1.00	9.42	6
ATOM	2864	C	ILE	A	351	24.372	20.509	18.459	1.00	7.26	6	ATOM	2917	CD2	TYR	A	358	22.294	24.466	28.799	1.00	9.67	6
ATOM	2865	O	ILE	A	351	23.668	20.349	19.498	1.00	7.46	8	ATOM	2918	CE2	TYR	A	358	21.900	25.783	29.085	1.00	9.55	6
ATOM	2866	H	LEU	A	352	23.960	21.213	17.423	1.00	7.13	7	ATOM	2919	CZ	TYR	A	358	21.466	26.587	28.050	1.00	9.41	6
ATOM	2867	CA	LEU	A	352	22.678	21.931	17.500	1.00	7.51	6	ATOM	2920	OH	TYR	A	358	21.076	27.879	28.304	1.00	8.90	8
ATOM	2868	CB	LEU	A	352	22.778	23.170	16.614	1.00	6.11	6	ATOM	2921	C	TYR	A	358	24.062	22.642	25.113	1.00	9.49	6
ATOM	2869	CG	LEU	A	352	23.789	24.248	17.000	1.00	7.70	6	ATOM	2922	O	TYR	A	358	25.195	22.737	25.552	1.00	9.20	8
ATOM	2870	CD1	LEU	A	352	23.973	25.292	15.878	1.00	6.26	6	ATOM	2923	N	PRO	A	359	23.809	22.981	23.858	1.00	9.59	7
ATOM	2871	CD2	LEU	A	352	23.307	24.932	18.273	1.00	6.10	6	ATOM	2924	CD	PRO	A	359	22.503	22.784	23.206	1.00	9.74	6
ATOM	2872	C	LEU	A	352	21.377	21.209	17.097	1.00	7.69	6	ATOM	2925	CA	PRO	A	359	24.786	23.481	22.907	1.00	9.51	6
ATOM	2873	O	LEU	A	352	20.314	21.664	17.512	1.00	7.18	8	ATOM	2926	CB	PRO	A	359	24.249	23.201	21.495	1.00	9.51	6
ATOM	2874	H	THR	A	353	21.530	20.143	16.291	1.00	8.22	7	ATOM	2927	CG	PRO	A	359	22.763	23.211	21.778	1.00	9.71	6
ATOM	2875	CA	THR	A	353	20.394	19.372	15.781	1.00	9.02	6	ATOM	2928	C	PRO	A	359	25.173	24.945	23.045	1.00	9.55	6
ATOM	2876	CB	THR	A	353	20.420	19.145	14.234	1.00	9.08	6	ATOM	2929	O	PRO	A	359	24.319	25.756	23.334	1.00	9.40	8
ATOM	2877	CG1	THR	A	353	21.434	18.262	13.784	1.00	8.55	8	ATOM	2930	N	GLN	A	360	26.454	25.242	22.837	1.00	9.58	7
ATOM	2878	CG2	THR	A	353	20.559	20.504	13.545	1.00	9.72	6	ATOM	2931	CA	GLN	A	360	26.970	26.588	22.963	1.00	9.76	6
ATOM	2879	C	THR	A	353	20.161	18.030	16.481	1.00	9.71	6	ATOM	2932	CB	GLN	A	360	28.115	26.660	24.024	1.00	11.01	6
ATOM	2880	O	THR	A	353	19.066	17.453	16.250	1.00	9.88	8	ATOM	2933	CG	GLN	A	360	30.427	27.709	25.524	1.00	14.42	8
ATOM	2881	H	ARG	A	354	21.086	17.601	17.369	1.00	10.05	7	ATOM	2934	CD	GLN	A	360	30.282	28.033	24.332	1.00	15.99	6
ATOM	2882	CA	ARG	A	354	20.883	16.330	18.085	1.00	10.58	6	ATOM	2935	OE1	GLN	A	360	30.427	27.709	25.524	1.00	14.42	8
ATOM	2883	CB	ARG	A	354	22.258	15.688	18.208	1.00	9.90	6	ATOM	2936	NE2	GLN	A	360	31.291	28.336	23.425	1.00	15.78	7
ATOM	2884	CG	ARG	A	354	22.706	15.117	16.879	1.00	8.76	6	ATOM	2937	C	GLN	A	360	27.481	27.096	21.610	1.00	9.39	6
ATOM	2885	CG	ARG	A	354	24.107	14.517	17.011	1.00	9.60	6	ATOM	2938	O	GLN	A	360	28.228	26.305	21.007	1.00	9.32	8
ATOM	2886	HE	ARG	A	354	24.016	13.348	17.864	1.00	8.67	7	ATOM	2939	N	VAL	A	361	27.111	28.317	21.278	1.00	9.24	7
ATOM	2887	CZ	ARG	A	354	23.434	12.222	17.541	1.00	9.03	6	ATOM	2940	CA	VAL	A	361	27.586	28.925	20.022	1.00	9.26	6
ATOM	2888	HN1	ARG	A	354	23.392	11.309	18.513	1.00	10.30	7	ATOM	2941	CB	VAL	A	361	26.532	29.709	19.230	1.00	10.17	6
ATOM	2889	HN2	ARG	A	354	22.866	11.890	16.408	1.00	8.32	7	ATOM	2942	CG1	VAL	A	361	27.159	30.437	18.039	1.00	9.02	6
ATOM	2890	C	ARG	A	354	20.103	16.563	19.378	1.00	11.10	6	ATOM	2943	CG2	VAL	A	361	25.394	28.761	18.785	1.00	9.34	6
ATOM	2891	O	ARG	A	354	20.157	17.713	19.854	1.00	11.27	8	ATOM	2944	C	VAL	A	361	28.739	29.880	20.354	1.00	9.12	6
ATOM	2892	N	GLU	A	355	19.325	15.618	19.921	1.00	11.22	7	ATOM	2945	O	VAL	A	361	28.526	30.595	21.350	1.00	9.34	8
ATOM	2893	CA	GLU	A	355	18.560	15.818	21.130	1.00	11.61	6	ATOM	2946	N	PIE	A	362	29.879	29.887	19.703	1.00	8.60	7
ATOM	2894	CB	GLU	A	355	17.527	14.661	21.351	1.00	14.92	6	ATOM	2947	CA	PIE	A	362	30.985	30.768	20.056	1.00	8.23	6
ATOM	2895	CG	GLU	A	355	18.229	13.320	21.567	1.00	17.30	6	ATOM	2948	CB	PIE	A	362	32.308	30.060	19.804	1.00	5.00	6
ATOM	2896	CD	GLU	A	355	17.370	12.087	21.646	1.00	19.96	6	ATOM	2949	CG	PIE	A	362	33.606	30.771	20.058	1.00	6.40	6
ATOM	2897	OE1	GLU	A	355	17.828	10.936	21.901	1.00	21.87	8	ATOM	2950	CD1	PIE	A	362	33.778	31.642	21.142	1.00	5.78	6
ATOM	2898	OE2	GLU	A	355	16.145	12.138	21.394	1.00	22.12	8	ATOM	2951	CD2	PIE	A	362	34.710	30.563	19.197	1.00	5.00	6
ATOM	2899	C	GLU	A	355	19.317	15.898	22.469	1.00	11.55	6	ATOM	2952	CE1	PIE	A	362	34.961	32.330	21.423	1.00	5.15	6
ATOM	2900	O	GLU	A	355	18.718	16.405	23.441	1.00	11.55	8	ATOM	2953	CE2	PIE	A	362	35.912	31.220	19.464	1.00	5.23	6
ATOM	2901	H	SER	A	356	20.569	15.450	22.576	1.00	11.30	7	ATOM	2954	CZ	PIE	A	362	36.039	32.080	20.579	1.00	5.49	6
ATOM	2902	CA	SER	A	356	21.130	15.577	23.939	1.00	11.56	6	ATOM	2955	C	PIE	A	362	30.967	32.053	19.251	1.00	8.28	6
ATOM	2903	CB	SER	A	356	21.398	14.171	24.475	1.00	13.81	6	ATOM	2956	O	PIE	A	362	30.857	32.004	18.043	1.00	7.85	8
ATOM	2904	CG	SER	A	356	22.246	13.514	23.552	1.00	18.62	8	ATOM	2957	N	TYR	A	363	31.117	33.210	19.872	1.00	8.47	7
ATOM	2905	C	SER	A	356	22.241	16.607	23.975	1.00	11.33	6	ATOM	2958	CA	TYR	A	363	31.144	34.545	19.289	1.00	8.84	6
ATOM	2906	O	SER	A	356	22.863	16.940	22.971	1.00	11.70	8	ATOM	2959	CB	TYR	A	363	31.363	35.652	20.344	1.00	9.13	6
ATOM	2907	N	GLY	A	357	22.426	17.219	25.136	1.00	10.87	7	ATOM	2960	CG	TYR	A	363	31.530	37.091	19.976	1.00	9.86	6
ATOM	2908	CA	GLY	A	357	23.363	18.269	25.422	1.00	10.39	6	ATOM	2961	CD1	TYR	A	363	30.479	37.981	20.213	1.00	10.09	6
ATOM	2909	C	GLY	A	357	22.619	19.622	25.239	1.00	10.36	6	ATOM	2962	CE1	TYR	A	363	30.585	39.317	19.904	1.00	10.35	6
ATOM	2910	O	GLY	A	357	21.602	19.837	24.547	1.00	10.17	8	ATOM	2963	CD2	TYR	A	363	32.709	37.609	19.410	1.00	10.25	6
ATOM	2911	N	TYR	A	358	23.255	20.608	25.880	1.00	10.01	7	ATOM	2964	CE2	TYR	A	363	32.850	38.956	19.091	1.00	10.30	6
ATOM	2912	CA	TYR	A	358	22.884	22.017	25.877	1.00	9.76	6	ATOM	2965	CZ	TYR	A	363	31.776	39.774	19.365	1.00	11.58	8
ATOM	2913	CB	TYR	A	358	22.669	22.498	27.311	1.00	9.60	6	ATOM	2966	OH	TYR	A	363	31.831	41.126	19.087	1.00	10.78	6
ATOM	2914	CG	TYR	A	358	22.268	23.937	27.516	1.00	9.61	6	ATOM	2967	C	TYR	A	363	32.241	34.680	18.187	1.00	8.73	6
ATOM	2915	CD1	TYR	A	358	21.829	24.775	26.494	1.00	9.48	6	ATOM	2968	O	TYR	A	363	32.011	35.363	17.191	1.00	8.42	8

2969	ATOM	H	GLY A 364	33.399	34.040	18.452	1.00	8.56	7
2970	ATOM	CA	GLY A 364	34.472	34.061	17.503	1.00	8.81	6
2971	ATOM	C	GLY A 364	34.083	33.261	16.231	1.00	9.04	6
2972	ATOM	O	GLY A 364	34.596	33.639	15.156	1.00	8.91	8
2973	ATOM	H	ASP A 365	33.233	32.251	16.327	1.00	9.21	7
2974	ATOM	CA	ASP A 365	32.830	31.513	15.137	1.00	9.93	6
2975	ATOM	CB	ASP A 365	32.255	30.146	15.429	1.00	8.93	6
2976	ATOM	CG	ASP A 365	33.369	29.235	15.977	1.00	9.58	6
2977	ATOM	001	ASP A 365	34.516	29.422	15.641	1.00	10.56	8
2978	ATOM	002	ASP A 365	33.078	28.275	16.700	1.00	9.75	8
2979	ATOM	C	ASP A 365	31.780	32.264	14.321	1.00	10.69	6
2980	ATOM	O	ASP A 365	30.887	32.135	13.078	1.00	10.75	8
2981	ATOM	H	HET A 366	31.770	32.996	14.980	1.00	11.93	7
2982	ATOM	CA	HET A 366	29.857	33.792	14.295	1.00	11.30	6
2983	ATOM	CB	HET A 366	28.838	34.351	15.303	1.00	14.14	6
2984	ATOM	CG	HET A 366	27.828	33.348	15.827	1.00	17.97	6
2985	ATOM	SD	HET A 366	26.475	33.032	14.646	1.00	22.02	16
2986	ATOM	CE	HET A 366	25.576	34.590	14.752	1.00	20.61	6
2987	ATOM	C	HET A 366	30.455	35.016	13.604	1.00	12.33	6
2988	ATOM	H	TYR A 367	30.240	35.367	12.445	1.00	12.31	8
2989	ATOM	CA	TYR A 367	31.249	35.740	14.417	1.00	12.74	7
2990	ATOM	CB	TYR A 367	31.831	36.964	13.927	1.00	13.46	6
2991	ATOM	CG	TYR A 367	31.548	38.065	14.988	1.00	14.31	6
2992	ATOM	CD1	TYR A 367	30.092	38.282	15.374	1.00	15.58	6
2993	ATOM	CD1	TYR A 367	29.721	38.284	16.730	1.00	15.98	6
2994	ATOM	CE1	TYR A 367	28.410	38.438	17.141	1.00	16.47	6
2995	ATOM	CE2	TYR A 367	29.075	38.425	14.433	1.00	16.06	6
2996	ATOM	CE2	TYR A 367	27.776	38.629	14.845	1.00	16.69	6
2997	ATOM	CZ	TYR A 367	27.431	38.644	16.196	1.00	16.89	6
2998	ATOM	OH	TYR A 367	26.105	38.815	16.553	1.00	16.92	8
2999	ATOM	C	TYR A 367	33.299	36.913	13.589	1.00	13.51	6
3000	ATOM	O	TYR A 367	33.733	38.005	13.190	1.00	13.49	8
3001	ATOM	H	GLY A 368	34.050	35.837	13.717	1.00	13.66	7
3002	ATOM	CA	GLY A 368	35.472	35.957	13.368	1.00	14.18	6
3003	ATOM	C	GLY A 368	36.289	36.369	14.599	1.00	14.83	6
3004	ATOM	O	GLY A 368	35.746	36.992	15.528	1.00	15.20	8
3005	ATOM	H	THR A 369	37.531	35.971	14.691	1.00	14.98	7
3006	ATOM	CA	THR A 369	38.409	36.330	15.759	1.00	15.75	6
3007	ATOM	CB	THR A 369	39.185	35.126	16.318	1.00	14.06	6
3008	ATOM	CG1	THR A 369	39.926	34.392	15.324	1.00	11.76	8
3009	ATOM	CG2	THR A 369	38.175	34.186	16.966	1.00	10.90	6
3010	ATOM	C	THR A 369	39.346	37.437	15.225	1.00	16.84	6
3011	ATOM	H	LYS A 370	39.727	37.463	14.039	1.00	16.53	8
3012	ATOM	O	LYS A 370	39.733	38.369	16.120	1.00	17.86	7
3013	ATOM	CA	LYS A 370	40.568	39.488	15.712	1.00	19.14	6
3014	ATOM	CB	LYS A 370	39.849	40.792	16.133	1.00	22.20	6
3015	ATOM	CG	LYS A 370	38.702	41.073	15.133	1.00	26.42	6
3016	ATOM	CD	LYS A 370	39.254	41.271	13.736	1.00	29.66	6
3017	ATOM	CE	LYS A 370	38.326	41.239	12.544	1.00	32.10	6
3018	ATOM	HZ	LYS A 370	39.111	41.178	11.243	1.00	33.93	7
3019	ATOM	C	LYS A 370	41.998	39.442	16.214	1.00	19.90	6
3020	ATOM	O	LYS A 370	42.638	40.436	16.526	1.00	19.78	8
3021	ATOM	N	GLY A 371	42.534	38.244	16.329	1.00	20.85	7
3022	ATOM	CA	GLY A 371	43.889	37.991	16.742	1.00	22.15	6
3023	ATOM	C	GLY A 371	44.817	38.443	15.581	1.00	23.36	6
3024	ATOM	O	GLY A 371	44.393	38.896	14.521	1.00	23.05	8
3025	ATOM	H	ASP A 372	46.095	38.223	15.877	1.00	24.83	7
3026	ATOM	CA	ASP A 372	47.186	38.626	15.016	1.00	26.55	6
3027	ATOM	CB	ASP A 372	48.323	39.306	15.874	1.00	31.39	6
3028	ATOM	CG	ASP A 372	47.962	40.791	15.968	1.00	37.36	8
3029	ATOM	001	ASP A 372	47.609	41.363	14.906	1.00	37.47	8
3030	ATOM	002	ASP A 372	47.972	41.443	17.034	1.00	37.31	6
3031	ATOM	C	ASP A 372	47.796	37.520	14.189	1.00	27.47	8
3032	ATOM	O	ASP A 372	48.870	37.818	13.613	1.00	27.65	8
3033	ATOM	H	SER A 373	47.162	36.353	14.146	1.00	27.64	7
3034	ATOM	CA	SER A 373	47.800	35.318	13.305	1.00	27.95	6
3035	ATOM	CB	SER A 373	47.678	33.936	13.932	1.00	26.91	6
3036	ATOM	CG	SER A 373	46.393	33.416	13.642	1.00	28.21	8
3037	ATOM	C	SER A 373	47.255	35.373	11.873	1.00	28.20	6
3038	ATOM	O	SER A 373	46.480	36.189	11.367	1.00	28.61	7
3039	ATOM	N	GLN A 374	47.780	34.393	11.137	1.00	28.86	6
3040	ATOM	CA	GLN A 374	47.348	34.201	9.729	1.00	28.86	6
3041	ATOM	CB	GLN A 374	48.525	34.112	8.767	1.00	40.44	6
3042	ATOM	CG	GLN A 374	49.400	35.309	8.530	1.00	40.44	6
3043	ATOM	CD	GLN A 374	48.939	36.714	8.874	1.00	45.21	6
3044	ATOM	OE1	GLN A 374	48.111	37.342	8.149	1.00	47.86	8
3045	ATOM	NE2	GLN A 374	49.449	37.277	10.005	1.00	45.97	7
3046	ATOM	C	GLN A 374	46.414	32.963	9.719	1.00	28.21	6
3047	ATOM	O	GLN A 374	46.105	32.340	8.674	1.00	28.76	8
3048	ATOM	N	ARG A 375	45.952	32.517	10.873	1.00	26.96	7
3049	ATOM	CA	ARG A 375	45.066	31.421	11.109	1.00	25.60	6
3050	ATOM	CB	ARG A 375	45.841	30.394	12.115	1.00	29.84	6
3051	ATOM	CG	ARG A 375	46.842	29.713	11.509	1.00	33.75	6
3052	ATOM	CD	ARG A 375	48.088	30.386	12.067	1.00	36.33	6
3053	ATOM	NE	ARG A 375	48.286	30.141	13.475	1.00	37.64	7
3054	ATOM	CZ	ARG A 375	47.856	29.261	14.351	1.00	37.09	6
3055	ATOM	HI1	ARG A 375	47.016	28.308	13.998	1.00	37.77	7
3056	ATOM	HI2	ARG A 375	48.293	29.399	15.587	1.00	36.83	7
3057	ATOM	C	ARG A 375	43.777	31.845	11.827	1.00	23.88	6
3058	ATOM	O	ARG A 375	43.218	30.942	12.450	1.00	23.81	8
3059	ATOM	H	GLU A 376	43.399	33.116	11.777	1.00	20.28	7
3060	ATOM	CA	GLU A 376	42.196	33.558	12.450	1.00	22.37	6
3061	ATOM	CB	GLU A 376	42.061	35.080	12.418	1.00	17.56	6
3062	ATOM	CG	GLU A 376	43.203	35.780	13.151	1.00	16.13	6
3063	ATOM	CD	GLU A 376	43.361	35.421	14.595	1.00	14.90	6
3064	ATOM	OE1	GLU A 376	42.403	35.436	15.391	1.00	12.95	8
3065	ATOM	OE2	GLU A 376	44.510	35.188	15.051	1.00	16.10	8
3066	ATOM	C	GLU A 376	40.955	32.886	11.869	1.00	19.17	6
3067	ATOM	O	GLU A 376	40.801	32.503	10.715	1.00	18.94	8
3068	ATOM	H	ILE A 377	40.002	32.698	12.777	1.00	18.23	7
3069	ATOM	CA	ILE A 377	38.726	32.102	12.410	1.00	17.23	6
3070	ATOM	CB	ILE A 377	37.924	31.634	13.636	1.00	15.28	6
3071	ATOM	CG1	ILE A 377	36.616	30.961	13.205	1.00	15.23	6
3072	ATOM	CG1	ILE A 377	38.720	30.715	14.564	1.00	14.23	6
3073	ATOM	CD1	ILE A 377	38.109	30.512	15.935	1.00	13.53	6
3074	ATOM	C	ILE A 377	37.957	33.184	11.660	1.00	16.78	6

ATOM	3075	O	ILE A 377	37.783	34.301	12.173	1.00	16.90	8	ATOM	3128	CO1	ILE A 384	28.029	28.790	12.411	1.00	13.70	6
ATOM	3076	H	PRO A 378	37.461	32.927	10.461	1.00	16.21	7	ATOM	3129	CO1	ILE A 384	28.902	29.649	13.343	1.00	15.12	6
ATOM	3077	CD	PRO A 378	37.634	31.617	9.821	1.00	16.04	6	ATOM	3130	C	ILE A 384	24.335	29.241	11.430	1.00	12.61	6
ATOM	3078	CA	PRO A 378	36.637	33.810	9.695	1.00	15.87	6	ATOM	3131	O	ILE A 384	23.621	28.363	11.931	1.00	12.68	8
ATOM	3079	CB	PRO A 378	36.555	33.232	8.263	1.00	15.98	6	ATOM	3132	N	GLU A 385	23.841	30.401	11.025	1.00	12.22	7
ATOM	3080	CG	PRO A 378	37.023	31.835	8.456	1.00	15.94	6	ATOM	3133	CA	GLU A 385	22.459	30.804	11.178	1.00	12.09	6
ATOM	3081	C	PRO A 378	35.214	33.860	10.247	1.00	15.56	6	ATOM	3134	CB	GLU A 385	22.249	32.252	10.671	1.00	13.25	6
ATOM	3082	O	PRO A 378	34.741	32.945	10.946	1.00	15.55	8	ATOM	3135	CG	GLU A 385	23.039	33.148	11.537	1.00	16.06	6
ATOM	3083	H	ALA A 379	34.506	34.960	9.931	1.00	15.19	7	ATOM	3136	CD	GLU A 385	22.681	34.621	11.631	1.00	18.04	6
ATOM	3084	CA	ALA A 379	33.095	35.063	10.370	1.00	14.83	6	ATOM	3137	OE1	GLU A 385	22.082	35.050	10.531	1.00	18.27	8
ATOM	3085	CB	ALA A 379	32.523	36.450	10.119	1.00	13.37	6	ATOM	3138	OE2	GLU A 385	22.960	35.427	12.453	1.00	18.60	8
ATOM	3086	C	ALA A 379	32.246	33.979	9.679	1.00	14.60	6	ATOM	3139	C	GLU A 385	21.439	29.867	10.587	1.00	11.96	6
ATOM	3087	O	ALA A 379	32.082	33.990	8.438	1.00	14.65	8	ATOM	3140	O	GLU A 385	20.439	29.608	11.273	1.00	12.04	8
ATOM	3088	H	LEU A 380	31.703	33.021	10.428	1.00	14.28	7	ATOM	3141	N	PRO A 386	21.614	29.238	9.436	1.00	11.74	7
ATOM	3089	CA	LEU A 380	30.925	31.960	9.792	1.00	14.14	6	ATOM	3142	CD	PRO A 386	22.735	29.467	8.528	1.00	11.74	6
ATOM	3090	CB	LEU A 380	31.468	30.617	10.265	1.00	15.00	6	ATOM	3143	CA	PRO A 386	20.676	28.265	8.905	1.00	11.52	6
ATOM	3091	CG	LEU A 380	32.913	30.303	9.865	1.00	16.56	6	ATOM	3144	CB	PRO A 386	21.205	27.847	7.516	1.00	11.54	6
ATOM	3092	CD1	LEU A 380	33.486	29.165	10.688	1.00	16.26	6	ATOM	3145	CG	PRO A 386	22.167	28.967	7.199	1.00	11.74	6
ATOM	3093	CD2	LEU A 380	32.975	30.004	8.350	1.00	16.68	6	ATOM	3146	C	PRO A 386	20.545	27.050	9.826	1.00	11.28	6
ATOM	3094	C	LEU A 380	29.448	32.123	10.017	1.00	14.34	6	ATOM	3147	O	PRO A 386	19.493	26.419	9.963	1.00	11.21	8
ATOM	3095	H	LYS A 381	28.602	31.262	9.773	1.00	14.38	8	ATOM	3148	N	ILE A 387	21.617	26.648	10.530	1.00	11.05	7
ATOM	3096	H	LYS A 381	29.011	33.278	10.475	1.00	14.36	7	ATOM	3149	CA	ILE A 387	21.619	25.492	11.424	1.00	10.84	6
ATOM	3097	CA	LYS A 381	27.615	33.579	10.719	1.00	14.84	6	ATOM	3150	CB	ILE A 387	23.047	24.957	11.653	1.00	8.79	6
ATOM	3098	CB	LYS A 381	27.672	35.101	10.820	1.00	18.02	6	ATOM	3151	CO2	ILE A 387	22.978	23.619	12.340	1.00	6.90	6
ATOM	3099	CG	LYS A 381	26.382	35.855	10.702	1.00	21.47	6	ATOM	3152	CG1	ILE A 387	23.799	24.850	10.310	1.00	8.27	6
ATOM	3100	CD	LYS A 381	26.754	37.314	10.944	1.00	25.20	6	ATOM	3153	CD1	ILE A 387	25.231	24.430	10.511	1.00	9.38	6
ATOM	3101	CE	LYS A 381	25.912	38.275	10.104	1.00	28.81	6	ATOM	3154	C	ILE A 387	20.917	25.808	12.754	1.00	11.01	6
ATOM	3102	NZ	LYS A 381	24.564	38.411	10.770	1.00	30.73	7	ATOM	3155	O	ILE A 387	20.273	24.946	13.366	1.00	10.92	8
ATOM	3103	C	LYS A 381	26.667	33.106	9.634	1.00	14.98	6	ATOM	3156	N	LEU A 388	21.058	27.064	13.176	1.00	11.09	7
ATOM	3104	O	LYS A 381	25.589	32.577	9.911	1.00	14.84	8	ATOM	3157	CA	LEU A 388	20.400	27.620	14.345	1.00	11.19	6
ATOM	3105	H	ILS A 382	26.978	33.273	8.350	1.00	14.98	7	ATOM	3158	CB	LEU A 388	20.902	29.010	14.682	1.00	10.46	6
ATOM	3106	CA	ILS A 382	26.079	32.889	7.268	1.00	15.22	6	ATOM	3159	CG	LEU A 388	22.084	29.061	15.638	1.00	11.84	6
ATOM	3107	CB	ILS A 382	26.562	33.593	5.986	1.00	21.24	6	ATOM	3160	CD1	LEU A 388	22.502	30.545	15.745	1.00	11.69	6
ATOM	3108	CG	ILS A 382	28.036	33.424	5.842	1.00	25.72	6	ATOM	3161	CD2	LEU A 388	21.636	28.377	16.916	1.00	10.70	6
ATOM	3109	CD2	ILS A 382	29.070	33.878	6.615	1.00	27.36	6	ATOM	3162	C	LEU A 388	18.887	27.688	14.042	1.00	11.21	6
ATOM	3110	HD1	ILS A 382	28.569	32.671	4.810	1.00	28.03	7	ATOM	3163	O	LEU A 388	18.017	27.443	14.899	1.00	11.36	8
ATOM	3111	CE1	ILS A 382	29.903	32.712	4.939	1.00	28.96	6	ATOM	3164	N	LYS A 389	18.551	28.015	12.792	1.00	11.22	7
ATOM	3112	NE2	ILS A 382	30.216	33.424	6.041	1.00	28.60	7	ATOM	3165	CA	LYS A 389	17.142	28.017	12.353	1.00	11.08	6
ATOM	3113	C	ILS A 382	25.947	31.415	7.118	1.00	15.05	6	ATOM	3166	CB	LYS A 389	17.014	28.553	10.952	1.00	14.65	6
ATOM	3114	O	ILS A 382	24.948	30.932	6.602	1.00	15.08	8	ATOM	3167	CG	LYS A 389	15.591	28.665	10.402	1.00	20.09	6
ATOM	3115	N	LYS A 383	26.887	30.595	7.622	1.00	14.81	7	ATOM	3168	CD	LYS A 389	15.454	30.134	9.985	1.00	24.33	6
ATOM	3116	CA	LYS A 383	26.802	29.161	7.615	1.00	14.36	6	ATOM	3169	CE	LYS A 389	14.860	30.232	8.592	1.00	27.30	6
ATOM	3117	CB	LYS A 383	28.186	28.551	7.528	1.00	16.14	6	ATOM	3170	NZ	LYS A 389	13.649	29.337	8.568	1.00	30.42	7
ATOM	3118	CG	LYS A 383	29.014	29.281	6.505	1.00	20.51	6	ATOM	3171	C	LYS A 389	16.620	26.566	12.377	1.00	10.52	6
ATOM	3119	CD	LYS A 383	29.147	28.507	5.230	1.00	23.48	6	ATOM	3172	O	LYS A 389	15.474	26.300	12.746	1.00	10.45	8
ATOM	3120	CE	LYS A 383	30.673	28.350	4.977	1.00	26.30	6	ATOM	3173	N	ALA A 390	17.445	25.613	11.937	1.00	10.03	7
ATOM	3121	NZ	LYS A 383	31.046	29.207	3.792	1.00	27.91	7	ATOM	3174	CA	ALA A 390	17.007	24.226	12.020	1.00	9.88	6
ATOM	3122	C	LYS A 383	26.207	28.595	8.926	1.00	13.88	6	ATOM	3175	CB	ALA A 390	17.970	23.263	11.375	1.00	7.86	6
ATOM	3123	O	LYS A 383	25.694	27.478	8.956	1.00	13.20	8	ATOM	3176	C	ALA A 390	16.848	23.832	13.506	1.00	9.86	6
ATOM	3124	N	ILE A 384	26.351	29.374	10.004	1.00	13.23	7	ATOM	3177	O	ALA A 390	15.876	23.103	13.761	1.00	9.92	8
ATOM	3125	CA	ILE A 384	25.814	28.889	11.252	1.00	12.99	6	ATOM	3178	N	ARG A 391	17.713	24.258	14.440	1.00	9.66	7
ATOM	3126	CB	ILE A 384	26.609	29.381	12.486	1.00	13.25	6	ATOM	3179	CA	ARG A 391	17.540	23.914	15.857	1.00	9.64	6
ATOM	3127	CG2	ILE A 384	25.905	29.000	13.778	1.00	12.19	6	ATOM	3180	CB	ARG A 391	18.666	24.410	16.800	1.00	8.27	6

ATOH	3181	CG	ARG A 391	18.295	24.255	18.295	1.00	6.17	6
ATOH	3182	CD	ARG A 391	19.637	24.301	19.079	1.00	6.11	6
ATOH	3183	ME	ARG A 391	19.415	23.982	20.476	1.00	6.39	7
ATOH	3184	CZ	ARG A 391	19.411	22.752	21.057	1.00	8.41	6
ATOH	3185	HH1	ARG A 391	19.671	21.719	20.264	1.00	7.01	7
ATOH	3186	HH2	ARG A 391	19.147	22.533	22.359	1.00	6.75	7
ATOH	3187	C	ARG A 391	16.258	24.518	16.434	1.00	9.84	6
ATOH	3188	O	ARG A 391	15.482	23.860	17.089	1.00	9.35	8
ATOH	3189	H	LYS A 392	16.061	25.811	16.184	1.00	10.42	7
ATOH	3190	CA	LYS A 392	14.904	26.555	16.666	1.00	11.31	6
ATOH	3191	CB	LYS A 392	15.137	28.036	16.253	1.00	13.27	6
ATOH	3192	CG	LYS A 392	14.066	28.928	16.797	1.00	16.07	6
ATOH	3193	CD	LYS A 392	14.176	30.388	16.369	1.00	20.09	6
ATOH	3194	CE	LYS A 392	12.806	31.069	16.665	1.00	23.10	6
ATOH	3195	HZ	LYS A 392	12.989	32.560	16.882	1.00	26.05	7
ATOH	3196	C	LYS A 392	13.536	26.046	16.200	1.00	11.94	6
ATOH	3197	O	LYS A 392	12.590	25.903	17.011	1.00	11.92	8
ATOH	3198	H	GLN A 393	12.091	25.218	14.916	1.00	12.38	7
ATOH	3199	CA	GLN A 393	11.736	25.947	14.386	1.00	12.80	6
ATOH	3200	CB	GLN A 393	12.463	27.237	12.917	1.00	24.67	6
ATOH	3201	CG	GLN A 393	11.701	28.402	12.316	1.00	29.33	6
ATOH	3202	CD	GLN A 393	11.924	28.717	11.149	1.00	30.64	8
ATOH	3203	OE1	GLN A 393	10.856	29.003	13.159	1.00	31.70	7
ATOH	3204	NE2	GLN A 393	11.921	23.764	13.940	1.00	12.57	6
ATOH	3205	C	GLN A 393	10.718	23.422	13.839	1.00	12.77	8
ATOH	3206	O	GLN A 394	12.995	23.041	13.678	1.00	11.99	7
ATOH	3207	H	TYR A 394	12.839	21.690	13.167	1.00	11.56	6
ATOH	3208	CA	TYR A 394	13.577	21.661	11.798	1.00	11.71	6
ATOH	3209	CB	TYR A 394	12.942	22.687	10.852	1.00	12.27	6
ATOH	3210	CG	TYR A 394	13.444	23.941	10.588	1.00	12.30	6
ATOH	3211	CD1	TYR A 394	12.811	24.826	9.747	1.00	12.61	6
ATOH	3212	CE1	TYR A 394	11.754	22.328	10.236	1.00	12.73	6
ATOH	3213	CD2	TYR A 394	11.066	23.192	9.378	1.00	13.02	6
ATOH	3214	CE2	TYR A 394	11.615	24.442	9.136	1.00	13.05	6
ATOH	3215	CZ	TYR A 394	10.942	25.224	8.229	1.00	13.25	8
ATOH	3216	OH	TYR A 394	13.360	20.552	14.017	1.00	11.27	6
ATOH	3217	C	TYR A 394	12.866	19.424	13.834	1.00	10.94	8
ATOH	3218	O	TYR A 394	14.338	20.794	14.908	1.00	10.88	7
ATOH	3219	H	ALA A 395	14.896	19.692	15.694	1.00	10.74	6
ATOH	3220	CA	ALA A 395	16.305	20.151	16.074	1.00	8.72	6
ATOH	3221	CB	ALA A 395	14.101	19.267	16.920	1.00	10.85	6
ATOH	3222	C	ALA A 395	14.392	19.591	18.082	1.00	10.94	8
ATOH	3223	O	ALA A 395	12.986	18.545	16.743	1.00	10.85	7
ATOH	3224	H	TYR A 396	12.061	18.070	17.753	1.00	10.83	6
ATOH	3225	CA	TYR A 396	10.763	18.949	17.821	1.00	10.80	6
ATOH	3226	CB	TYR A 396	11.083	20.390	18.180	1.00	10.52	6
ATOH	3227	CG	TYR A 396	11.333	21.365	17.195	1.00	10.49	6
ATOH	3228	CD1	TYR A 396	11.683	22.665	17.546	1.00	10.23	6
ATOH	3229	CE1	TYR A 396	11.215	20.744	19.504	1.00	10.24	6
ATOH	3230	CD2	TYR A 396	11.536	22.043	19.835	1.00	10.18	6
ATOH	3231	CE2	TYR A 396	11.799	22.984	18.874	1.00	10.23	6
ATOH	3232	CZ	TYR A 396	12.200	24.237	19.305	1.00	10.59	8
ATOH	3233	OH	TYR A 396						
ATOH	3234	C	TYR A 396	11.624	16.631	17.499	1.00	10.90	6
ATOH	3235	O	TYR A 396	11.615	16.137	16.372	1.00	10.58	8
ATOH	3236	N	GLY A 397	11.252	15.899	18.555	1.00	11.07	7
ATOH	3237	CA	GLY A 397	10.772	14.542	18.296	1.00	11.32	6
ATOH	3238	C	GLY A 397	11.808	13.450	18.353	1.00	11.58	6
ATOH	3239	O	GLY A 397	13.001	13.761	18.466	1.00	12.00	8
ATOH	3240	N	ALA A 398	11.341	12.228	18.304	1.00	11.57	7
ATOH	3241	CA	ALA A 398	12.172	11.044	18.341	1.00	11.80	6
ATOH	3242	CB	ALA A 398	11.261	9.824	18.105	1.00	9.85	6
ATOH	3243	C	ALA A 398	13.348	11.115	17.365	1.00	12.04	6
ATOH	3244	O	ALA A 398	13.259	11.447	16.176	1.00	12.09	8
ATOH	3245	N	GLN A 399	14.532	10.718	17.833	1.00	12.00	7
ATOH	3246	CA	GLN A 399	15.761	10.691	17.058	1.00	12.04	6
ATOH	3247	CB	GLN A 399	16.871	11.357	17.912	1.00	10.48	6
ATOH	3248	CG	GLN A 399	18.261	11.287	17.366	1.00	9.54	6
ATOH	3249	CD	GLN A 399	19.195	12.269	18.066	1.00	9.97	6
ATOH	3250	OE1	GLN A 399	18.983	13.467	18.191	1.00	8.29	8
ATOH	3251	NE2	GLN A 399	20.306	11.751	18.528	1.00	9.30	7
ATOH	3252	C	GLN A 399	16.212	9.307	16.643	1.00	12.27	6
ATOH	3253	O	GLN A 399	16.138	8.327	17.361	1.00	12.29	8
ATOH	3254	N	HIS A 400	16.765	9.135	15.415	1.00	12.36	7
ATOH	3255	CA	HIS A 400	17.270	7.893	14.903	1.00	12.28	6
ATOH	3256	CB	HIS A 400	16.419	7.243	13.800	1.00	12.34	6
ATOH	3257	CG	HIS A 400	15.001	6.998	14.252	1.00	13.76	6
ATOH	3258	CD2	HIS A 400	14.464	6.087	15.135	1.00	12.53	6
ATOH	3259	ND1	HIS A 400	13.959	7.856	13.831	1.00	13.34	7
ATOH	3260	CE1	HIS A 400	12.860	7.408	14.435	1.00	11.97	6
ATOH	3261	NE2	HIS A 400	13.095	6.378	15.194	1.00	11.69	7
ATOH	3262	C	HIS A 400	18.710	8.179	14.411	1.00	12.21	6
ATOH	3263	O	HIS A 400	18.909	9.132	13.670	1.00	11.78	8
ATOH	3264	N	ASP A 401	19.651	7.332	14.895	1.00	12.31	7
ATOH	3265	CA	ASP A 401	21.043	7.503	14.536	1.00	12.71	6
ATOH	3266	CB	ASP A 401	21.964	7.308	15.758	1.00	15.32	6
ATOH	3267	CG	ASP A 401	21.883	8.427	16.767	1.00	18.10	6
ATOH	3268	CD1	ASP A 401	21.438	9.578	16.520	1.00	20.24	8
ATOH	3269	CD2	ASP A 401	22.299	8.187	17.921	1.00	19.29	8
ATOH	3270	C	ASP A 401	21.556	6.515	13.484	1.00	12.57	6
ATOH	3271	O	ASP A 401	21.145	5.360	13.483	1.00	12.31	8
ATOH	3272	N	TYR A 402	22.385	6.972	12.584	1.00	12.55	7
ATOH	3273	CA	TYR A 402	22.977	6.173	11.524	1.00	12.83	6
ATOH	3274	CB	TYR A 402	22.385	6.495	10.130	1.00	12.68	6
ATOH	3275	CG	TYR A 402	20.891	6.179	10.105	1.00	12.98	6
ATOH	3276	CD1	TYR A 402	19.990	7.186	10.470	1.00	13.23	6
ATOH	3277	CE1	TYR A 402	18.631	6.952	10.544	1.00	13.64	6
ATOH	3278	CD2	TYR A 402	20.378	4.927	9.801	1.00	13.10	6
ATOH	3279	CE2	TYR A 402	19.018	4.654	9.819	1.00	13.39	6
ATOH	3280	CZ	TYR A 402	18.168	5.676	10.195	1.00	14.02	6
ATOH	3281	OH	TYR A 402	16.795	5.502	10.282	1.00	14.72	8
ATOH	3282	C	TYR A 402	26.478	6.371	11.592	1.00	13.30	6
ATOH	3283	O	TYR A 402	25.019	7.054	10.747	1.00	13.17	8
ATOH	3284	N	PIE A 403	25.162	5.818	12.581	1.00	14.08	7
ATOH	3285	CA	PIE A 403	26.591	5.861	12.792	1.00	14.73	6
ATOH	3286	CB	PIE A 403	26.978	6.035	14.266	1.00	16.26	6

ATOH	3287	CG	PIIE A 403	26.766	7.486	14.665	1.00	19.71	6	ATOH	3340	CA	VAL A 409	27.012	9.436	9.309	1.00	11.68	6
ATOH	3288	CD1	PIIE A 403	25.574	7.927	15.176	1.00	20.07	6	ATOH	3341	CB	VAL A 409	27.735	9.616	10.638	1.00	13.02	6
ATOH	3289	CD2	PIIE A 403	27.748	8.440	14.583	1.00	21.01	6	ATOH	3342	CG1	VAL A 409	28.916	8.661	10.804	1.00	14.14	6
ATOH	3290	CE1	PIIE A 403	25.379	9.241	15.534	1.00	21.71	6	ATOH	3343	CG2	VAL A 409	28.293	11.030	10.817	1.00	11.59	6
ATOH	3291	CE2	PIIE A 403	27.540	9.786	14.804	1.00	22.26	6	ATOH	3344	C	VAL A 409	25.823	10.380	9.245	1.00	11.38	6
ATOH	3292	CZ	PIIE A 403	26.338	10.216	15.345	1.00	21.47	6	ATOH	3345	O	VAL A 409	25.887	11.441	8.613	1.00	11.38	8
ATOH	3293	C	PIIE A 403	27.113	4.537	12.220	1.00	15.16	6	ATOH	3346	N	GLY A 410	24.747	10.000	9.898	1.00	10.96	7
ATOH	3294	O	PIIE A 403	27.616	3.625	12.902	1.00	15.23	8	ATOH	3347	CA	GLY A 410	23.548	10.842	9.910	1.00	10.41	6
ATOH	3295	H	ASP A 404	26.987	4.370	10.906	1.00	15.33	7	ATOH	3348	C	GLY A 410	22.635	10.508	11.084	1.00	9.89	6
ATOH	3296	CA	ASP A 404	27.398	3.103	10.294	1.00	15.59	6	ATOH	3349	O	GLY A 410	22.871	9.547	11.830	1.00	9.68	8
ATOH	3297	CB	ASP A 404	26.115	2.428	9.754	1.00	17.33	6	ATOH	3350	N	TRP A 411	21.623	11.347	11.201	1.00	9.60	7
ATOH	3298	CG	ASP A 404	25.433	3.431	8.838	1.00	19.38	6	ATOH	3351	CA	TRP A 411	20.569	11.201	12.204	1.00	9.34	6
ATOH	3299	CD1	ASP A 404	25.870	4.570	8.544	1.00	19.96	8	ATOH	3352	CB	TRP A 411	20.994	11.750	13.574	1.00	8.12	6
ATOH	3300	CD2	ASP A 404	24.330	3.060	8.407	1.00	21.24	8	ATOH	3353	CG	TRP A 411	21.417	13.213	13.561	1.00	8.50	6
ATOH	3301	C	ASP A 404	28.346	3.116	9.119	1.00	15.47	6	ATOH	3354	CD2	TRP A 411	22.726	13.662	13.285	1.00	8.48	6
ATOH	3302	O	ASP A 404	28.339	2.154	8.320	1.00	15.71	8	ATOH	3355	CE2	TRP A 411	22.699	15.049	13.356	1.00	8.47	6
ATOH	3303	N	HIS A 405	29.168	4.144	8.997	1.00	15.11	7	ATOH	3356	CE3	TRP A 411	23.924	13.010	12.971	1.00	9.18	6
ATOH	3304	CA	HIS A 405	30.098	4.238	7.885	1.00	14.80	6	ATOH	3357	CD1	TRP A 411	20.647	14.285	13.808	1.00	6.27	6
ATOH	3305	CB	HIS A 405	29.332	4.915	6.719	1.00	14.80	6	ATOH	3358	NE1	TRP A 411	21.483	15.439	13.671	1.00	6.58	7
ATOH	3306	CG	HIS A 405	30.187	4.926	5.492	1.00	15.21	6	ATOH	3359	CZ2	TRP A 411	23.830	15.839	13.113	1.00	9.15	6
ATOH	3307	CD2	HIS A 405	30.385	3.954	4.561	1.00	15.68	6	ATOH	3360	CZ3	TRP A 411	25.054	13.814	12.732	1.00	9.35	6
ATOH	3308	HD1	HIS A 405	30.992	5.990	5.157	1.00	15.84	7	ATOH	3361	CH2	TRP A 411	25.007	15.163	12.799	1.00	9.69	6
ATOH	3309	CE1	HIS A 405	31.654	5.723	4.041	1.00	16.58	6	ATOH	3362	C	TRP A 411	19.296	11.897	11.708	1.00	9.23	6
ATOH	3310	NE2	HIS A 405	31.309	4.491	3.680	1.00	17.15	7	ATOH	3363	O	TRP A 411	19.372	12.824	10.901	1.00	8.76	9
ATOH	3311	C	HIS A 405	31.280	5.023	8.383	1.00	14.46	6	ATOH	3364	N	THR A 412	18.151	11.418	12.226	1.00	9.36	7
ATOH	3312	O	HIS A 405	31.008	5.908	9.197	1.00	14.63	8	ATOH	3365	CA	THR A 412	16.877	12.015	11.894	1.00	9.69	6
ATOH	3313	N	HIS A 406	32.494	4.841	7.963	1.00	14.11	7	ATOH	3366	CB	THR A 412	15.968	11.081	11.040	1.00	10.82	6
ATOH	3314	CA	HIS A 406	33.630	5.587	8.495	1.00	13.78	6	ATOH	3367	CG1	THR A 412	15.687	9.914	11.826	1.00	12.10	8
ATOH	3315	CB	HIS A 406	35.000	4.932	8.189	1.00	15.67	6	ATOH	3368	CG2	THR A 412	16.614	10.613	9.743	1.00	9.28	6
ATOH	3316	CG	HIS A 406	34.981	4.416	6.777	1.00	16.76	6	ATOH	3369	C	THR A 412	16.136	12.441	13.173	1.00	9.93	6
ATOH	3317	CD2	HIS A 406	34.450	3.265	6.232	1.00	16.51	6	ATOH	3370	O	THR A 412	16.399	12.027	14.318	1.00	9.78	8
ATOH	3318	HD1	HIS A 406	35.504	5.164	5.733	1.00	18.12	7	ATOH	3371	N	ARG A 413	15.184	13.348	12.978	1.00	10.07	7
ATOH	3319	CE1	HIS A 406	35.318	4.505	4.578	1.00	16.95	6	ATOH	3372	CA	ARG A 413	14.332	13.843	14.055	1.00	10.74	6
ATOH	3320	NE2	HIS A 406	34.666	3.388	4.880	1.00	17.55	7	ATOH	3373	CB	ARG A 413	14.635	15.236	14.615	1.00	8.23	6
ATOH	3321	C	HIS A 406	33.580	7.002	8.026	1.00	13.47	6	ATOH	3374	CG	ARG A 413	16.039	15.382	15.182	1.00	6.55	6
ATOH	3322	O	HIS A 406	34.298	7.753	8.672	1.00	13.10	8	ATOH	3375	CD	ARG A 413	16.262	14.604	16.464	1.00	6.58	6
ATOH	3323	N	ASP A 407	32.861	7.500	7.048	1.00	13.42	7	ATOH	3376	NE	ARG A 413	15.388	14.982	17.577	1.00	5.58	7
ATOH	3324	CA	ASP A 407	32.837	8.877	6.628	1.00	13.27	6	ATOH	3377	CZ	ARG A 413	15.602	16.062	18.326	1.00	8.01	6
ATOH	3325	CB	ASP A 407	33.163	9.063	5.138	1.00	14.59	6	ATOH	3378	HH1	ARG A 413	14.802	16.370	19.349	1.00	7.49	7
ATOH	3326	CG	ASP A 407	34.556	8.665	4.654	1.00	16.13	6	ATOH	3379	HH2	ARG A 413	16.645	16.870	18.094	1.00	7.65	7
ATOH	3327	CD1	ASP A 407	35.474	8.360	5.486	1.00	14.23	8	ATOH	3380	C	ARG A 413	12.946	13.767	13.403	1.00	11.41	6
ATOH	3328	CD2	ASP A 407	34.808	8.646	3.381	1.00	18.38	8	ATOH	3381	O	ARG A 413	12.678	14.374	12.355	1.00	11.24	8
ATOH	3329	C	ASP A 407	31.457	9.532	6.757	1.00	12.98	6	ATOH	3382	N	GLU A 414	12.076	12.980	14.035	1.00	12.08	7
ATOH	3330	O	ASP A 407	31.310	10.601	7.360	1.00	12.77	8	ATOH	3383	CA	GLU A 414	10.713	12.785	13.510	1.00	12.84	6
ATOH	3331	N	ILE A 408	30.465	8.890	6.167	1.00	12.85	7	ATOH	3384	CB	GLU A 414	9.957	11.626	14.195	1.00	11.98	6
ATOH	3332	CA	ILE A 408	29.098	9.438	6.133	1.00	12.79	6	ATOH	3385	CG	GLU A 414	10.578	10.270	13.880	1.00	12.67	6
ATOH	3333	CB	ILE A 408	28.429	9.103	4.799	1.00	14.07	6	ATOH	3386	CD	GLU A 414	9.722	9.123	14.401	1.00	14.64	6
ATOH	3334	CG1	ILE A 408	27.045	9.742	4.656	1.00	12.86	6	ATOH	3387	OE1	GLU A 414	8.485	9.240	14.504	1.00	14.73	8
ATOH	3335	CG2	ILE A 408	29.251	9.578	3.597	1.00	13.69	6	ATOH	3388	OE2	GLU A 414	10.249	8.041	14.723	1.00	15.78	8
ATOH	3336	CD1	ILE A 408	28.979	8.781	2.321	1.00	14.63	6	ATOH	3389	C	GLU A 414	9.819	14.015	13.605	1.00	13.32	6
ATOH	3337	C	ILE A 408	28.219	8.885	7.260	1.00	12.60	6	ATOH	3390	O	GLU A 414	8.855	14.006	12.864	1.00	13.17	8
ATOH	3338	O	ILE A 408	27.838	7.712	7.271	1.00	12.81	8	ATOH	3391	N	GLY A 415	10.096	15.006	14.389	1.00	14.06	7
ATOH	3339	N	VAL A 409	27.910	9.762	8.195	1.00	12.05	7	ATOH	3392	CA	GLY A 415	9.223	16.150	14.467	1.00	15.71	6

ATOH	3393	C	GLY A 415	8.276	15.870	15.637	1.00	17.18	6	ATOH	3446	CA	LEU A 424	14.738	16.900	9.939	1.00	10.33	6
ATOH	3394	O	GLY A 415	8.176	14.768	16.148	1.00	17.23	8	ATOH	3447	CB	LEU A 424	15.547	18.024	10.607	1.00	7.87	6
ATOH	3395	H	ASP A 416	7.581	16.904	16.048	1.00	18.70	7	ATOH	3448	CG	LEU A 424	16.337	17.716	11.885	1.00	8.31	6
ATOH	3396	CA	ASP A 416	6.606	16.860	17.118	1.00	20.18	6	ATOH	3449	CD1	LEU A 424	17.570	16.854	11.716	1.00	6.65	6
ATOH	3397	CB	ASP A 416	7.228	17.531	18.307	1.00	26.49	6	ATOH	3450	CD2	LEU A 424	16.682	19.107	12.547	1.00	8.33	6
ATOH	3398	CG	ASP A 416	6.358	17.615	19.535	1.00	31.33	6	ATOH	3451	C	LEU A 424	15.577	15.630	9.701	1.00	10.11	6
ATOH	3399	OO1	ASP A 416	6.791	18.402	20.413	1.00	35.28	8	ATOH	3452	O	LEU A 424	15.448	14.626	10.407	1.00	10.06	8
ATOH	3400	OO2	ASP A 416	5.301	16.975	19.696	1.00	32.88	8	ATOH	3453	N	ALA A 425	16.469	15.658	8.706	1.00	9.69	7
ATOH	3401	C	ASP A 416	5.400	17.597	16.568	1.00	21.08	6	ATOH	3454	CA	ALA A 425	17.366	14.563	8.361	1.00	9.38	6
ATOH	3402	O	ASP A 416	5.423	18.631	15.908	1.00	20.94	8	ATOH	3455	CB	ALA A 425	16.885	13.742	7.143	1.00	6.73	6
ATOH	3403	H	SER A 417	4.234	17.031	16.824	1.00	22.16	7	ATOH	3456	C	ALA A 425	18.723	15.226	8.124	1.00	9.43	6
ATOH	3404	CA	SER A 417	2.928	17.484	16.380	1.00	23.18	6	ATOH	3457	O	ALA A 425	18.868	16.069	7.188	1.00	9.26	8
ATOH	3405	CB	SER A 417	1.868	16.471	16.846	1.00	27.52	6	ATOH	3458	N	ALA A 426	19.705	14.875	8.971	1.00	9.31	7
ATOH	3406	OG	SER A 417	1.734	16.874	18.237	1.00	32.78	8	ATOH	3459	CA	ALA A 426	21.016	15.474	8.873	1.00	9.28	6
ATOH	3407	C	SER A 417	2.585	18.852	16.929	1.00	23.50	6	ATOH	3460	CB	ALA A 426	21.436	16.104	10.234	1.00	9.50	6
ATOH	3408	O	SER A 417	1.821	19.541	16.258	1.00	23.90	8	ATOH	3461	C	ALA A 426	22.032	14.435	8.414	1.00	9.49	6
ATOH	3409	H	SER A 418	3.145	19.217	18.073	1.00	23.61	6	ATOH	3462	O	ALA A 426	21.989	13.294	8.823	1.00	9.20	8
ATOH	3410	CA	SER A 418	2.982	20.541	18.628	1.00	24.90	6	ATOH	3463	N	LEU A 427	22.965	14.846	7.581	1.00	9.84	7
ATOH	3411	CB	SER A 418	3.247	20.523	20.135	1.00	27.24	8	ATOH	3464	CA	LEU A 427	24.057	14.016	7.090	1.00	10.53	6
ATOH	3412	OG	SER A 418	4.660	20.195	20.198	1.00	27.24	8	ATOH	3465	CB	LEU A 427	23.734	13.630	5.656	1.00	11.90	6
ATOH	3413	C	SER A 418	3.988	21.525	18.023	1.00	23.37	6	ATOH	3466	CG	LEU A 427	23.768	12.238	5.062	1.00	13.08	6
ATOH	3414	O	SER A 418	3.995	22.714	18.503	1.00	23.96	8	ATOH	3467	CD1	LEU A 427	23.577	11.104	6.058	1.00	11.36	6
ATOH	3415	H	VAL A 419	4.894	21.195	17.094	1.00	22.44	7	ATOH	3468	CD2	LEU A 427	22.742	12.170	3.946	1.00	12.77	6
ATOH	3416	CA	VAL A 419	5.793	22.233	16.490	1.00	21.33	6	ATOH	3469	C	LEU A 427	25.327	14.877	7.098	1.00	10.73	6
ATOH	3417	CB	VAL A 419	7.278	22.269	16.815	1.00	19.53	6	ATOH	3470	O	LEU A 427	25.367	16.056	6.700	1.00	10.84	8
ATOH	3418	CG1	VAL A 419	8.070	23.317	16.038	1.00	15.95	6	ATOH	3471	N	ILE A 428	26.460	14.404	7.520	1.00	10.83	7
ATOH	3419	CG2	VAL A 419	7.558	22.527	18.315	1.00	18.97	6	ATOH	3472	CA	ILE A 428	27.758	15.045	7.515	1.00	11.06	6
ATOH	3420	C	VAL A 419	5.477	21.951	14.988	1.00	20.67	6	ATOH	3473	CB	ILE A 428	28.190	15.609	8.889	1.00	11.39	6
ATOH	3421	O	VAL A 419	5.911	20.939	14.404	1.00	20.45	8	ATOH	3474	CG2	ILE A 428	27.289	16.778	9.305	1.00	10.31	6
ATOH	3422	H	ALA A 420	4.616	22.803	14.400	1.00	20.01	7	ATOH	3475	CG1	ILE A 428	28.230	14.513	9.993	1.00	9.31	6
ATOH	3423	CA	ALA A 420	4.174	22.558	13.017	1.00	19.28	6	ATOH	3476	CD1	ILE A 428	28.912	15.018	11.283	1.00	8.18	6
ATOH	3424	CB	ALA A 420	3.189	23.619	12.527	1.00	19.92	6	ATOH	3477	C	ILE A 428	28.779	14.006	6.996	1.00	11.33	6
ATOH	3425	C	ALA A 420	5.329	23.619	12.527	1.00	18.43	6	ATOH	3478	O	ILE A 428	28.561	12.780	7.210	1.00	11.63	8
ATOH	3426	O	ALA A 420	6.221	23.297	12.166	1.00	17.67	7	ATOH	3479	N	THR A 429	29.881	14.325	6.326	1.00	11.15	7
ATOH	3427	N	ASH A 421	5.312	21.471	11.161	1.00	17.67	7	ATOH	3480	CA	THR A 429	30.873	13.403	5.891	1.00	10.98	6
ATOH	3428	CA	ASH A 421	6.356	21.242	10.168	1.00	16.69	6	ATOH	3481	CB	THR A 429	31.176	13.138	4.393	1.00	11.90	6
ATOH	3429	CB	ASH A 421	6.537	22.436	9.204	1.00	19.20	6	ATOH	3482	OG1	THR A 429	30.085	13.558	3.592	1.00	14.12	8
ATOH	3430	CG	ASH A 421	5.312	22.617	8.330	1.00	21.29	6	ATOH	3483	CG2	THR A 429	31.612	11.738	4.125	1.00	8.62	6
ATOH	3431	OO1	ASH A 421	4.586	21.711	7.966	1.00	22.05	8	ATOH	3484	C	THR A 429	32.246	14.119	6.111	1.00	10.97	6
ATOH	3432	ND2	ASH A 421	5.028	23.853	7.994	1.00	23.75	7	ATOH	3485	O	THR A 429	32.413	15.275	5.717	1.00	10.27	8
ATOH	3433	C	ASH A 421	7.760	20.891	10.703	1.00	15.64	6	ATOH	3486	N	ASP A 430	33.213	13.328	6.605	1.00	11.50	7
ATOH	3434	O	ASN A 421	8.711	20.946	9.931	1.00	15.23	8	ATOH	3487	CA	ASP A 430	34.560	13.968	6.672	1.00	11.94	6
ATOH	3435	N	SER A 422	7.882	20.479	11.947	1.00	14.78	7	ATOH	3488	CB	ASP A 430	35.391	13.652	7.861	1.00	11.35	6
ATOH	3436	CA	SER A 422	9.140	20.088	12.542	1.00	14.31	6	ATOH	3489	CG	ASP A 430	35.704	12.175	7.893	1.00	12.16	6
ATOH	3437	CB	SER A 422	9.064	20.137	14.071	1.00	16.37	6	ATOH	3490	OO1	ASP A 430	34.941	11.410	7.236	1.00	12.11	8
ATOH	3438	OG	SER A 422	7.990	19.345	14.623	1.00	13.80	8	ATOH	3491	OO2	ASP A 430	36.676	11.784	8.551	1.00	10.98	8
ATOH	3439	C	SER A 422	9.518	18.705	12.009	1.00	13.67	6	ATOH	3492	C	ASP A 430	35.289	13.562	5.390	1.00	12.62	6
ATOH	3440	N	SER A 422	8.713	17.932	11.459	1.00	13.79	8	ATOH	3493	O	ASP A 430	36.452	13.961	5.293	1.00	12.99	8
ATOH	3441	H	GLY A 423	10.797	18.389	12.161	1.00	12.94	7	ATOH	3494	N	GLY A 431	34.710	12.876	4.425	1.00	12.92	7
ATOH	3442	CA	GLY A 423	11.329	17.086	11.679	1.00	12.05	6	ATOH	3495	CA	GLY A 431	35.369	12.496	3.173	1.00	13.60	6
ATOH	3443	C	GLY A 423	12.546	17.472	10.825	1.00	11.56	6	ATOH	3496	C	GLY A 431	34.447	12.693	1.981	1.00	13.93	6
ATOH	3444	O	GLY A 423	12.532	18.566	10.232	1.00	11.46	8	ATOH	3497	O	GLY A 431	33.681	13.671	1.929	1.00	13.86	8
ATOH	3445	N	LEU A 424	13.562	16.612	10.738	1.00	10.94	7	ATOH	3498	N	PRO A 432	34.509	11.820	0.999	1.00	14.36	7

ATOH	3499	CD	PRO A 432	35.409	10.665	0.884	1.00	14.46	6	ATOH	3552	CD2	TYR A 439	11.815	5.768	11.397	1.00	16.76	6
ATOH	3500	CA	PRO A 432	33.653	11.935	-0.199	1.00	14.68	6	ATOH	3553	CE2	TYR A 439	10.514	5.667	11.875	1.00	17.07	6
ATOH	3501	CB	PRO A 432	34.035	10.827	-1.190	1.00	14.46	6	ATOH	3554	C2	TYR A 439	9.490	5.433	10.974	1.00	17.36	6
ATOH	3502	CG	PRO A 432	35.224	10.168	-0.544	1.00	14.43	6	ATOH	3555	OH	TYR A 439	8.184	5.345	11.408	1.00	17.36	8
ATOH	3503	C	PRO A 432	32.163	11.902	0.220	1.00	14.96	6	ATOH	3556	C	TYR A 439	13.404	8.144	9.357	1.00	15.81	6
ATOH	3504	O	PRO A 432	31.795	11.354	1.273	1.00	14.84	8	ATOH	3557	O	TYR A 439	13.994	8.512	10.382	1.00	15.50	8
ATOH	3505	H	GLY A 433	31.312	12.512	-0.641	1.00	15.15	7	ATOH	3558	H	VAL A 440	12.407	8.831	8.856	1.00	16.08	7
ATOH	3506	CA	GLY A 433	29.882	12.569	-0.450	1.00	15.39	6	ATOH	3559	CA	VAL A 440	11.897	10.144	9.350	1.00	16.61	6
ATOH	3507	C	GLY A 433	29.192	11.254	-0.788	1.00	15.65	6	ATOH	3560	CB	VAL A 440	11.999	10.905	7.980	1.00	16.77	6
ATOH	3508	O	GLY A 433	29.814	10.259	-1.188	1.00	15.62	8	ATOH	3561	CG1	VAL A 440	10.764	11.601	7.561	1.00	17.08	6
ATOH	3509	H	GLY A 434	27.885	11.213	-0.658	1.00	15.83	7	ATOH	3562	CG2	VAL A 440	13.263	11.754	8.026	1.00	15.70	6
ATOH	3510	CA	GLY A 434	27.160	9.983	-0.950	1.00	15.94	6	ATOH	3563	C	VAL A 440	10.554	10.106	10.031	1.00	17.07	6
ATOH	3511	C	GLY A 434	25.733	10.059	-0.444	1.00	15.96	6	ATOH	3564	O	VAL A 440	10.014	11.040	10.625	1.00	16.85	8
ATOH	3512	O	GLY A 434	25.263	11.153	-0.176	1.00	16.25	8	ATOH	3565	N	GLY A 441	9.900	8.915	9.995	1.00	17.47	7
ATOH	3513	H	ALA A 435	25.080	8.825	-0.297	1.00	15.72	7	ATOH	3566	CA	GLY A 441	8.807	8.729	10.597	1.00	18.13	6
ATOH	3514	CA	ALA A 435	23.722	8.972	0.128	1.00	15.72	6	ATOH	3567	C	GLY A 441	7.583	8.699	9.476	1.00	18.60	6
ATOH	3515	CB	ALA A 435	22.858	8.337	-1.047	1.00	15.08	6	ATOH	3568	O	GLY A 441	7.616	9.450	8.514	1.00	18.47	8
ATOH	3516	C	ALA A 435	23.470	7.942	1.309	1.00	15.68	6	ATOH	3569	H	ARG A 442	6.636	7.793	9.673	1.00	19.21	7
ATOH	3517	O	ALA A 435	24.260	7.007	1.516	1.00	15.51	8	ATOH	3570	CA	ARG A 442	5.540	7.559	8.739	1.00	19.79	6
ATOH	3518	H	LYS A 436	22.366	8.252	2.019	1.00	15.52	7	ATOH	3571	CB	ARG A 442	4.804	6.264	9.145	1.00	27.13	6
ATOH	3519	CA	LYS A 436	21.990	7.383	3.119	1.00	15.58	6	ATOH	3572	CG	ARG A 442	3.910	5.788	8.008	1.00	34.25	6
ATOH	3520	CB	LYS A 436	22.566	7.682	4.490	1.00	15.09	6	ATOH	3573	CD	ARG A 442	3.727	4.252	7.911	1.00	40.05	6
ATOH	3521	CG	LYS A 436	22.500	6.476	5.442	1.00	14.85	6	ATOH	3574	HE	ARG A 442	3.027	3.980	6.634	1.00	44.01	7
ATOH	3522	CD	LYS A 436	23.071	6.769	6.810	1.00	13.83	6	ATOH	3575	CZ	ARG A 442	1.896	3.329	6.388	1.00	46.30	6
ATOH	3523	CE	LYS A 436	24.448	7.441	6.784	1.00	12.21	6	ATOH	3576	HN1	ARG A 442	1.175	2.772	7.381	1.00	47.10	7
ATOH	3524	NZ	LYS A 436	25.498	6.400	6.652	1.00	11.33	7	ATOH	3577	HN2	ARG A 442	1.446	3.253	5.119	1.00	46.98	7
ATOH	3525	C	LYS A 436	20.447	7.396	3.179	1.00	15.62	6	ATOH	3578	C	ARG A 442	4.586	8.725	8.657	1.00	19.53	6
ATOH	3526	O	LYS A 436	19.778	8.405	3.060	1.00	15.33	8	ATOH	3579	O	ARG A 442	3.955	9.003	7.621	1.00	19.67	8
ATOH	3527	H	ARG A 437	19.931	6.177	3.314	1.00	15.95	7	ATOH	3580	N	GLN A 443	4.479	9.544	9.684	1.00	19.05	7
ATOH	3528	CA	ARG A 437	18.502	5.972	3.422	1.00	16.36	6	ATOH	3581	CA	GLN A 443	3.607	10.709	9.658	1.00	18.69	6
ATOH	3529	CB	ARG A 437	17.965	4.624	2.977	1.00	23.29	6	ATOH	3582	CB	GLN A 443	3.431	11.246	11.093	1.00	21.29	6
ATOH	3530	CG	ARG A 437	17.573	4.499	1.510	1.00	29.80	6	ATOH	3583	CG	GLN A 443	4.808	11.675	11.634	1.00	23.26	6
ATOH	3531	CD	ARG A 437	16.656	3.293	1.407	1.00	35.68	6	ATOH	3584	CD	GLN A 443	5.581	10.603	12.390	1.00	24.64	6
ATOH	3532	NE	ARG A 437	15.201	3.525	1.319	1.00	40.60	7	ATOH	3585	OE1	GLN A 443	5.631	9.402	12.134	1.00	24.10	8
ATOH	3533	CE	ARG A 437	14.309	2.734	1.964	1.00	42.03	6	ATOH	3586	NE2	GLN A 443	6.316	11.066	13.438	1.00	25.50	7
ATOH	3534	HN1	ARG A 437	14.735	1.740	2.755	1.00	42.08	7	ATOH	3587	C	GLN A 443	4.115	11.806	8.734	1.00	18.06	6
ATOH	3535	HN2	ARG A 437	13.005	2.950	1.814	1.00	42.49	7	ATOH	3588	O	GLN A 443	3.414	12.798	8.501	1.00	17.90	8
ATOH	3536	C	ARG A 437	18.202	6.050	4.911	1.00	15.94	6	ATOH	3589	H	ASN A 444	5.307	11.714	8.193	1.00	17.51	7
ATOH	3537	O	ARG A 437	18.833	5.318	5.678	1.00	15.62	8	ATOH	3590	CA	ASN A 444	5.897	12.636	7.253	1.00	16.84	6
ATOH	3538	H	HET A 438	17.303	6.932	5.265	1.00	15.86	7	ATOH	3591	CB	ASN A 444	7.400	12.828	7.563	1.00	14.89	6
ATOH	3539	CA	HET A 438	17.019	7.059	6.722	1.00	15.87	6	ATOH	3592	CG	ASN A 444	7.497	13.458	8.951	1.00	15.66	6
ATOH	3540	CB	HET A 438	17.846	8.236	7.242	1.00	16.35	6	ATOH	3593	CO1	ASN A 444	6.765	14.374	9.269	1.00	13.70	8
ATOH	3541	CG	HET A 438	19.360	8.200	7.266	1.00	15.99	6	ATOH	3594	ND2	ASN A 444	8.368	12.974	9.818	1.00	15.53	7
ATOH	3542	SD	HET A 438	20.172	9.634	7.987	1.00	16.66	16	ATOH	3595	C	ASN A 444	5.814	12.078	5.820	1.00	16.45	6
ATOH	3543	CE	HET A 438	19.698	10.989	6.970	1.00	14.67	6	ATOH	3596	O	ASN A 444	6.396	12.716	4.943	1.00	16.24	8
ATOH	3544	C	HET A 438	15.525	7.205	6.983	1.00	15.63	6	ATOH	3597	N	ALA A 445	5.196	10.917	5.640	1.00	16.01	7
ATOH	3545	O	HET A 438	14.774	7.662	6.109	1.00	15.49	8	ATOH	3598	H	ALA A 445	5.075	10.268	4.345	1.00	16.03	6
ATOH	3546	H	TYR A 439	15.065	6.827	8.145	1.00	15.53	7	ATOH	3599	CB	ALA A 445	4.109	9.075	4.403	1.00	15.55	6
ATOH	3547	CA	TYR A 439	13.699	6.862	8.590	1.00	15.72	6	ATOH	3600	C	ALA A 445	4.572	11.159	3.208	1.00	15.90	6
ATOH	3548	CB	TYR A 439	13.484	5.632	9.498	1.00	15.96	6	ATOH	3601	O	ALA A 445	3.624	11.896	3.441	1.00	15.97	8
ATOH	3549	CG	TYR A 439	12.110	5.576	10.071	1.00	16.56	6	ATOH	3602	N	GLY A 446	5.165	11.130	2.010	1.00	15.77	7
ATOH	3550	CO1	TYR A 439	11.044	5.338	9.188	1.00	17.21	6	ATOH	3603	CA	GLY A 446	4.752	11.944	0.885	1.00	15.36	6
ATOH	3551	CE1	TYR A 439	9.728	5.283	9.611	1.00	17.34	6	ATOH	3604	C	GLY A 446	5.207	13.378	0.863	1.00	15.20	6

ATOM	3605	O	GLY A 446	4.924	14.124	-0.086	1.00	15.33	8	ATOM	3658	CG1	ILE A 452	17.009	25.640	6.443	1.00	14.27	6
ATOM	3606	N	GLU A 447	5.963	13.897	1.827	1.00	14.73	7	ATOM	3659	CD1	ILE A 452	16.275	25.551	7.802	1.00	14.37	6
ATOM	3607	CA	GLU A 447	6.387	15.280	1.807	1.00	14.28	6	ATOM	3660	C	ILE A 452	19.424	26.911	4.512	1.00	13.90	6
ATOM	3608	CB	GLU A 447	6.706	15.729	3.264	1.00	14.39	6	ATOM	3661	O	ILE A 452	19.482	26.146	4.529	1.00	13.78	8
ATOM	3609	CG	GLU A 447	5.389	15.838	4.018	1.00	13.77	6	ATOM	3662	N	THR A 453	20.598	24.254	4.476	1.00	14.31	7
ATOM	3610	CD	GLU A 447	5.715	15.992	5.455	1.00	15.49	6	ATOM	3663	CA	THR A 453	21.885	24.911	4.427	1.00	14.90	6
ATOM	3611	OE1	GLU A 447	6.875	16.135	5.959	1.00	15.55	8	ATOM	3664	CB	THR A 453	23.063	23.977	4.697	1.00	12.74	6
ATOM	3612	OE2	GLU A 447	4.721	16.000	6.203	1.00	15.31	8	ATOM	3665	OG1	THR A 453	23.194	23.019	3.614	1.00	12.38	8
ATOM	3613	C	GLU A 447	7.644	16.838	1.041	1.00	13.72	6	ATOM	3666	CG2	THR A 453	22.905	23.215	6.001	1.00	12.32	6
ATOM	3614	O	GLU A 447	8.494	16.838	0.929	1.00	13.70	8	ATOM	3667	O	THR A 453	22.184	25.480	3.030	1.00	15.80	6
ATOM	3615	N	THR A 448	7.703	16.924	0.604	1.00	13.28	7	ATOM	3668	O	THR A 453	23.073	26.280	2.774	1.00	15.75	8
ATOM	3616	CA	THR A 448	8.904	17.386	-0.059	1.00	13.29	6	ATOM	3669	N	GLY A 454	21.475	24.968	2.016	1.00	16.49	7
ATOM	3617	CB	THR A 448	8.681	18.432	-1.179	1.00	14.50	6	ATOM	3670	CA	GLY A 454	21.614	25.345	0.622	1.00	16.88	6
ATOM	3618	OG1	THR A 448	9.966	18.972	-1.787	1.00	12.12	6	ATOM	3671	C	GLY A 454	22.752	24.598	-0.055	1.00	17.42	6
ATOM	3619	CG2	THR A 448	9.826	18.047	0.994	1.00	12.85	6	ATOM	3672	O	GLY A 454	22.967	24.858	-1.237	1.00	17.55	8
ATOM	3620	C	THR A 448	9.440	19.036	1.627	1.00	12.61	8	ATOM	3673	N	ASN A 455	23.496	23.700	0.568	1.00	17.19	6
ATOM	3621	O	THR A 448	11.021	17.500	1.176	1.00	12.53	7	ATOM	3674	CA	ASN A 455	24.590	22.992	-0.090	1.00	18.19	6
ATOM	3622	N	TRP A 449	12.011	18.069	2.095	1.00	12.56	6	ATOM	3675	CG	ASN A 455	25.375	22.188	0.928	1.00	17.61	6
ATOM	3623	CA	TRP A 449	12.564	16.992	3.035	1.00	9.67	6	ATOM	3676	CG	ASN A 455	26.145	23.158	1.831	1.00	19.02	6
ATOM	3624	CB	TRP A 449	11.619	16.660	4.133	1.00	9.33	6	ATOM	3677	OO1	ASN A 455	26.584	24.193	1.296	1.00	20.84	8
ATOM	3625	CG	TRP A 449	11.959	16.118	5.402	1.00	8.65	6	ATOM	3678	NO2	ASN A 455	26.283	22.827	3.103	1.00	17.34	7
ATOM	3626	CD2	TRP A 449	10.762	15.974	6.129	1.00	9.46	6	ATOM	3679	C	ASN A 455	24.050	22.108	-1.217	1.00	18.75	6
ATOM	3627	CE2	TRP A 449	13.161	15.756	6.000	1.00	9.00	6	ATOM	3680	O	ASN A 455	24.847	21.968	-2.160	1.00	18.87	8
ATOM	3628	CE3	TRP A 449	10.237	16.787	4.154	1.00	9.60	6	ATOM	3681	N	ARG A 456	22.843	21.544	-1.115	1.00	18.85	7
ATOM	3629	CD1	TRP A 449	9.710	16.414	5.351	1.00	9.39	7	ATOM	3682	CA	ARG A 456	22.300	20.763	-2.215	1.00	19.42	6
ATOM	3630	NE1	TRP A 449	10.730	15.465	7.438	1.00	9.93	6	ATOM	3683	CG	ARG A 456	22.051	19.313	-1.853	1.00	21.00	6
ATOM	3631	C22	TRP A 449	13.135	15.216	7.286	1.00	7.79	6	ATOM	3684	CB	ARG A 456	23.405	18.670	-1.612	1.00	22.06	6
ATOM	3632	C23	TRP A 449	11.953	15.068	7.958	1.00	8.43	6	ATOM	3685	CD	ARG A 456	23.079	17.230	-1.408	1.00	24.47	6
ATOM	3633	CH2	TRP A 449	13.168	18.721	1.320	1.00	12.82	6	ATOM	3686	HE	ARG A 456	22.752	16.607	-2.676	1.00	27.86	7
ATOM	3634	C	TRP A 449	13.563	18.178	0.275	1.00	12.56	8	ATOM	3687	C2	ARG A 456	23.472	16.017	-3.613	1.00	29.09	6
ATOM	3635	N	HS A 450	13.727	19.836	1.779	1.00	13.04	7	ATOM	3688	HH1	ARG A 456	22.809	15.484	-4.631	1.00	29.42	7
ATOM	3636	CA	HS A 450	14.852	20.452	1.046	1.00	13.34	6	ATOM	3689	HH2	ARG A 456	24.789	15.821	-3.652	1.00	30.25	7
ATOM	3637	CG	HS A 450	14.296	21.682	0.331	1.00	14.62	6	ATOM	3690	C	ARG A 456	20.994	21.388	-2.721	1.00	19.69	6
ATOM	3638	CB	HS A 450	14.289	22.883	1.191	1.00	17.87	6	ATOM	3691	O	ARG A 456	20.182	21.809	-1.881	1.00	19.86	8
ATOM	3639	CG	HS A 450	14.806	24.101	1.061	1.00	19.94	6	ATOM	3692	N	SER A 457	20.777	21.515	-4.032	1.00	19.78	7
ATOM	3640	CD2	HS A 450	13.580	22.945	2.378	1.00	20.15	7	ATOM	3693	CA	SER A 457	19.533	22.134	-4.501	1.00	19.97	6
ATOM	3641	HD1	HS A 450	13.725	24.121	2.973	1.00	20.37	6	ATOM	3694	CB	SER A 457	19.748	23.040	-5.741	1.00	20.18	6
ATOM	3642	CE1	HS A 450	14.513	24.848	2.189	1.00	21.15	7	ATOM	3695	OG	SER A 457	20.301	22.068	-6.668	1.00	20.86	8
ATOM	3643	HE2	HS A 450	16.040	20.732	1.990	1.00	13.31	6	ATOM	3696	C	SER A 457	18.439	21.136	-4.883	1.00	19.94	6
ATOM	3644	C	HS A 450	15.781	20.891	3.188	1.00	13.10	8	ATOM	3697	O	SER A 457	17.317	21.592	-5.183	1.00	20.17	8
ATOM	3645	O	HS A 450	17.301	20.807	1.520	1.00	13.09	7	ATOM	3698	N	GLU A 458	18.708	19.841	-4.835	1.00	19.72	7
ATOM	3646	N	ASP A 451	18.454	21.055	2.375	1.00	12.90	6	ATOM	3699	CA	GLU A 458	17.687	18.883	-5.161	1.00	19.82	6
ATOM	3647	CB	ASP A 451	19.697	20.740	1.535	1.00	10.89	6	ATOM	3700	CG	GLU A 458	18.321	17.611	-5.803	1.00	24.71	6
ATOM	3648	CA	ASP A 451	21.008	21.054	3.391	1.00	10.97	6	ATOM	3701	CG	GLU A 458	17.134	17.001	-6.543	1.00	31.90	6
ATOM	3649	CG	ASP A 451	20.976	21.407	3.391	1.00	9.94	8	ATOM	3702	CD	GLU A 458	17.152	15.635	-7.168	1.00	36.18	6
ATOM	3650	OO1	ASP A 451	22.111	20.978	1.592	1.00	11.53	8	ATOM	3703	OE1	GLU A 458	18.250	15.229	-7.681	1.00	38.60	8
ATOM	3651	OO2	ASP A 451	18.403	22.477	2.886	1.00	13.21	6	ATOM	3704	OE2	GLU A 458	16.057	14.979	-7.142	1.00	38.01	8
ATOM	3652	C	ASP A 451	18.643	23.419	2.089	1.00	13.23	8	ATOM	3705	C	GLU A 458	16.850	17.778	-3.978	1.00	19.28	6
ATOM	3653	O	ASP A 451	18.095	22.816	4.131	1.00	13.24	7	ATOM	3706	O	GLU A 458	17.375	17.778	-3.068	1.00	19.23	8
ATOM	3654	N	ILE A 452	17.466	24.235	4.561	1.00	13.53	6	ATOM	3707	CD	PRO A 459	15.545	18.628	-4.028	1.00	18.75	7
ATOM	3655	CA	ILE A 452	17.466	24.250	5.994	1.00	13.03	6	ATOM	3708	N	PRO A 459	14.893	19.401	-5.083	1.00	18.49	6
ATOM	3656	CB	ILE A 452	18.495	23.677	6.964	1.00	11.72	6	ATOM	3709	CA	PRO A 459	14.611	18.231	-2.974	1.00	18.56	6
ATOM	3657	CG2	ILE A 452							ATOM	3710	CB	PRO A 459	13.270	18.916	-3.298	1.00	18.40	6

ATOM	3711	CG	PRO A 459	13.637	19.885	-4.393	1.00	18.37	6	ATOM	3764	CA	TRP A 467	11.860	6.686	4.486	1.00	20.35	6
ATOM	3712	C	PRO A 459	14.504	16.723	-2.839	1.00	18.47	6	ATOM	3765	CB	TRP A 467	12.439	5.313	4.107	1.00	20.44	6
ATOM	3713	O	PRO A 459	14.829	15.979	-3.780	1.00	18.68	8	ATOM	3766	CG	TRP A 467	12.372	4.283	5.181	1.00	20.04	6
ATOM	3714	N	VAL A 460	14.113	16.146	-1.728	1.00	18.24	7	ATOM	3767	CD2	TRP A 467	13.427	3.771	5.993	1.00	19.41	6
ATOM	3715	CA	VAL A 460	13.987	14.691	-1.504	1.00	18.19	6	ATOM	3768	CE2	TRP A 467	12.844	2.826	6.880	1.00	19.61	6
ATOM	3716	CB	VAL A 460	14.906	14.168	-0.379	1.00	17.56	6	ATOM	3769	CE3	TRP A 467	14.803	3.987	6.049	1.00	18.58	6
ATOM	3717	CG1	VAL A 460	12.685	12.685	-0.076	1.00	17.48	6	ATOM	3770	CD1	TRP A 467	11.227	3.633	5.591	1.00	20.26	6
ATOM	3718	CG2	VAL A 460	16.371	14.396	-0.750	1.00	17.31	6	ATOM	3771	NE1	TRP A 467	11.497	2.779	6.622	1.00	19.67	7
ATOM	3719	C	VAL A 460	12.528	14.396	-1.209	1.00	18.23	6	ATOM	3772	CE2	TRP A 467	13.593	2.102	7.824	1.00	19.59	6
ATOM	3720	O	VAL A 460	11.892	15.157	-0.428	1.00	18.51	8	ATOM	3773	CE3	TRP A 467	15.552	3.268	6.997	1.00	20.04	6
ATOM	3721	N	VAL A 461	11.894	13.362	-1.798	1.00	18.03	7	ATOM	3774	CE2	TRP A 467	14.959	2.315	7.868	1.00	19.86	6
ATOM	3722	CA	VAL A 461	10.468	13.105	-1.458	1.00	17.66	6	ATOM	3775	C	TRP A 467	12.174	7.631	3.312	1.00	20.06	6
ATOM	3723	CB	VAL A 461	9.584	12.863	-2.709	1.00	17.06	6	ATOM	3776	O	TRP A 467	11.355	7.837	2.413	1.00	19.99	8
ATOM	3724	CG1	VAL A 461	8.143	12.564	-2.256	1.00	16.42	6	ATOM	3777	N	GLY A 468	13.356	8.193	3.372	1.00	19.55	7
ATOM	3725	CG2	VAL A 461	9.629	14.023	-3.678	1.00	15.12	6	ATOM	3778	CA	GLY A 468	13.838	9.105	2.345	1.00	19.08	6
ATOM	3726	C	VAL A 461	10.418	11.943	-0.456	1.00	17.45	6	ATOM	3779	C	GLY A 468	15.293	8.667	2.044	1.00	18.67	6
ATOM	3727	O	VAL A 461	11.046	10.893	-0.596	1.00	17.01	8	ATOM	3780	O	GLY A 468	15.969	8.121	2.908	1.00	18.51	8
ATOM	3728	N	ILE A 462	9.707	12.111	0.647	1.00	17.69	7	ATOM	3781	N	GLU A 469	15.761	8.896	0.848	1.00	18.42	7
ATOM	3729	CA	ILE A 462	9.596	11.050	1.642	1.00	18.12	6	ATOM	3782	CA	GLU A 469	17.153	8.577	0.487	1.00	18.35	6
ATOM	3730	CB	ILE A 462	9.212	11.549	3.046	1.00	15.81	6	ATOM	3783	CG	GLU A 469	17.287	7.714	-0.771	1.00	23.55	6
ATOM	3731	CG2	ILE A 462	9.222	10.334	3.984	1.00	15.11	6	ATOM	3784	CG	GLU A 469	18.710	7.626	-1.293	1.00	29.59	6
ATOM	3732	CG1	ILE A 462	10.089	12.691	3.597	1.00	13.00	6	ATOM	3785	CD	GLU A 469	18.967	7.178	-2.729	1.00	34.28	6
ATOM	3733	CD1	ILE A 462	11.575	12.439	3.642	1.00	9.27	6	ATOM	3786	OE1	GLU A 469	19.831	6.252	-2.904	1.00	36.09	8
ATOM	3734	C	ILE A 462	8.554	10.036	1.116	1.00	18.85	6	ATOM	3787	OE2	GLU A 469	18.340	7.755	-3.681	1.00	35.52	8
ATOM	3735	O	ILE A 462	7.432	10.390	0.717	1.00	18.67	8	ATOM	3788	C	GLU A 469	17.805	9.964	0.424	1.00	17.57	6
ATOM	3736	N	ASN A 463	8.922	8.755	1.138	1.00	19.55	7	ATOM	3789	O	GLU A 469	17.555	10.801	-0.433	1.00	17.46	8
ATOM	3737	CA	ASN A 463	8.090	7.650	0.672	1.00	20.49	6	ATOM	3790	N	PHE A 470	18.666	10.297	1.388	1.00	17.09	7
ATOM	3738	CB	ASN A 463	8.960	6.443	0.342	1.00	20.20	6	ATOM	3791	CA	PHE A 470	19.246	11.660	1.415	1.00	16.47	6
ATOM	3739	CG	ASN A 463	9.411	5.430	1.361	1.00	21.59	6	ATOM	3792	CB	PHE A 470	19.076	12.181	2.850	1.00	14.77	6
ATOM	3740	OD1	ASN A 463	9.117	5.376	2.570	1.00	22.11	8	ATOM	3793	CG	PHE A 470	17.686	12.126	3.451	1.00	11.90	6
ATOM	3741	NO2	ASN A 463	10.221	4.455	0.904	1.00	19.99	7	ATOM	3794	CD1	PHE A 470	17.301	11.041	4.208	1.00	11.94	6
ATOM	3742	C	ASN A 463	6.975	7.297	1.630	1.00	21.45	6	ATOM	3795	CD2	PHE A 470	16.823	13.197	3.296	1.00	10.16	6
ATOM	3743	O	ASN A 463	6.884	7.742	2.770	1.00	21.42	8	ATOM	3796	CE1	PHE A 470	16.037	11.030	4.790	1.00	11.36	6
ATOM	3744	N	SER A 464	6.070	6.390	1.173	1.00	22.31	7	ATOM	3797	CE2	PHE A 470	15.562	13.155	3.871	1.00	9.61	6
ATOM	3745	CA	SER A 464	4.877	5.971	1.916	1.00	22.97	6	ATOM	3798	CZ	PHE A 470	15.159	12.069	4.605	1.00	9.27	6
ATOM	3746	CB	SER A 464	3.915	5.159	1.024	1.00	23.92	6	ATOM	3799	C	PHE A 470	20.682	11.731	0.945	1.00	16.14	6
ATOM	3747	OG	SER A 464	4.365	3.841	0.731	1.00	25.69	8	ATOM	3800	O	PHE A 470	21.406	10.761	1.154	1.00	16.37	8
ATOM	3748	C	SER A 464	5.187	5.303	3.248	1.00	23.29	6	ATOM	3801	N	HIS A 471	21.142	12.807	0.363	1.00	15.78	7
ATOM	3749	O	SER A 464	4.319	5.400	4.131	1.00	23.52	8	ATOM	3802	CA	HIS A 471	22.462	13.007	-0.146	1.00	15.69	6
ATOM	3750	N	GLU A 465	6.344	4.722	3.486	1.00	23.46	7	ATOM	3803	CB	HIS A 471	22.332	13.373	-1.655	1.00	17.00	6
ATOM	3751	CA	GLU A 465	6.814	4.134	4.708	1.00	23.73	6	ATOM	3804	CG	HIS A 471	21.894	12.216	-2.515	1.00	20.58	6
ATOM	3752	CB	GLU A 465	7.931	3.164	4.313	1.00	29.98	6	ATOM	3805	CD2	HIS A 471	22.588	11.406	-3.372	1.00	21.49	6
ATOM	3753	CG	GLU A 465	7.852	1.671	4.515	1.00	35.99	6	ATOM	3806	NO1	HIS A 471	20.560	11.780	-2.567	1.00	22.05	7
ATOM	3754	CD	GLU A 465	6.542	1.117	3.976	1.00	39.49	6	ATOM	3807	CE1	HIS A 471	20.481	10.745	-3.399	1.00	21.74	6
ATOM	3755	OE1	GLU A 465	6.407	1.177	2.734	1.00	41.43	8	ATOM	3808	NE2	HIS A 471	21.688	10.491	-3.900	1.00	22.49	7
ATOM	3756	OE2	GLU A 465	5.709	0.684	4.812	1.00	41.76	8	ATOM	3809	C	HIS A 471	23.282	14.111	0.504	1.00	15.47	6
ATOM	3757	C	GLU A 465	7.511	5.095	5.721	1.00	23.27	6	ATOM	3810	O	HIS A 471	22.727	15.102	0.997	1.00	15.28	8
ATOM	3758	O	GLU A 465	7.857	4.672	6.848	1.00	23.24	8	ATOM	3811	N	VAL A 472	24.618	13.993	0.466	1.00	15.23	7
ATOM	3759	N	GLY A 466	7.744	6.345	5.324	1.00	22.53	7	ATOM	3812	CA	VAL A 472	25.529	14.978	0.964	1.00	15.01	6
ATOM	3760	CA	GLY A 466	8.436	7.317	6.135	1.00	21.95	6	ATOM	3813	CG	VAL A 472	26.385	14.698	2.271	1.00	16.48	6
ATOM	3761	C	GLY A 466	9.969	7.245	5.909	1.00	21.47	6	ATOM	3814	CB1	VAL A 472	26.201	15.727	3.368	1.00	15.07	6
ATOM	3762	O	GLY A 466	10.728	7.644	6.820	1.00	21.33	8	ATOM	3815	CG2	VAL A 472	26.275	13.274	2.750	1.00	17.23	6
ATOM	3763	N	TRP A 467	10.441	6.770	4.751	1.00	20.79	7	ATOM	3816	C	VAL A 472	26.730	15.205	0.001	1.00	14.42	6

ATOH	3817	O	VAL A 472	27.246	14.169	-0.462	1.00	14.29	8
ATOH	3818	N	ASH A 473	27.200	16.444	-0.101	1.00	13.78	7
ATOH	3819	CA	ASH A 473	28.404	16.662	-0.901	1.00	13.30	6
ATOH	3820	CB	ASH A 473	28.514	18.108	-1.339	1.00	13.44	6
ATOH	3821	CG	ASH A 473	27.403	18.519	-2.301	1.00	15.11	6
ATOH	3822	OO1	ASH A 473	26.781	17.637	-2.882	1.00	15.07	8
ATOH	3823	NO2	ASH A 473	27.148	19.805	-2.494	1.00	15.52	7
ATOH	3824	C	ASH A 473	29.633	16.278	-0.086	1.00	12.99	6
ATOH	3825	O	ASH A 473	29.567	16.164	1.139	1.00	12.88	7
ATOH	3826	H	GLY A 474	30.792	16.046	-0.723	1.00	12.57	7
ATOH	3827	CA	GLY A 474	32.004	15.690	0.026	1.00	11.90	6
ATOH	3828	C	GLY A 474	32.429	16.874	0.897	1.00	11.47	6
ATOH	3829	O	GLY A 474	32.305	18.054	0.524	1.00	11.68	8
ATOH	3830	H	GLY A 475	32.940	16.534	2.058	1.00	10.93	7
ATOH	3831	CA	GLY A 475	33.425	17.392	3.139	1.00	10.37	6
ATOH	3832	C	GLY A 475	32.350	18.425	3.486	1.00	10.04	6
ATOH	3833	O	GLY A 475	32.646	19.606	3.607	1.00	9.82	8
ATOH	3834	H	SER A 476	31.076	17.953	3.556	1.00	9.71	7
ATOH	3835	CA	SER A 476	29.967	18.862	3.748	1.00	9.25	6
ATOH	3836	CB	SER A 476	29.330	19.038	2.348	1.00	10.16	6
ATOH	3837	OG	SER A 476	28.487	20.170	2.237	1.00	11.03	8
ATOH	3838	C	SER A 476	28.910	18.374	4.718	1.00	8.87	6
ATOH	3839	O	SER A 477	28.982	17.301	5.311	1.00	8.60	8
ATOH	3840	N	VAL A 477	27.865	19.207	4.864	1.00	8.73	7
ATOH	3841	CA	VAL A 477	26.711	18.975	5.699	1.00	8.42	6
ATOH	3842	CB	VAL A 477	26.705	19.802	7.028	1.00	6.94	6
ATOH	3843	CG1	VAL A 477	26.953	21.281	6.811	1.00	5.00	6
ATOH	3844	CG2	VAL A 477	25.462	19.333	7.754	1.00	5.67	6
ATOH	3845	C	VAL A 477	25.485	20.297	4.139	1.00	8.35	6
ATOH	3846	O	VAL A 477	24.403	18.567	5.033	1.00	8.26	8
ATOH	3847	H	SER A 478	23.087	18.761	4.462	1.00	8.36	6
ATOH	3848	CA	SER A 478	22.792	17.840	3.254	1.00	8.85	6
ATOH	3849	CB	SER A 478	23.251	18.520	2.073	1.00	11.98	8
ATOH	3850	OG	SER A 478	22.074	18.493	5.574	1.00	8.16	6
ATOH	3851	C	SER A 478	22.181	17.527	6.326	1.00	7.79	8
ATOH	3852	O	SER A 478	21.114	19.406	5.720	1.00	8.43	7
ATOH	3853	N	ILE A 479	20.039	19.323	6.693	1.00	8.49	6
ATOH	3854	CA	ILE A 479	20.160	20.274	7.884	1.00	8.78	6
ATOH	3855	CB	ILE A 479	18.976	19.999	8.846	1.00	6.48	6
ATOH	3856	CG2	ILE A 479	21.502	20.102	8.647	1.00	8.82	6
ATOH	3857	CG1	ILE A 479	21.914	21.342	9.399	1.00	7.53	6
ATOH	3858	CO1	ILE A 479	18.689	19.539	6.015	1.00	8.75	6
ATOH	3859	C	ILE A 479	18.346	20.671	5.734	1.00	8.75	6
ATOH	3860	O	ILE A 479	17.969	18.447	5.791	1.00	9.32	7
ATOH	3861	N	TYR A 480	16.682	18.457	5.141	1.00	10.04	6
ATOH	3862	CA	TYR A 480	16.431	17.093	4.465	1.00	10.47	6
ATOH	3863	CB	TYR A 480	17.358	16.901	3.299	1.00	11.51	6
ATOH	3864	CG	TYR A 480	18.620	16.314	3.605	1.00	12.15	6
ATOH	3865	CO1	TYR A 480	19.531	16.102	2.589	1.00	12.53	6
ATOH	3866	CE1	TYR A 480	17.080	17.306	2.001	1.00	11.63	6
ATOH	3867	CE2	TYR A 480	17.988	17.112	0.996	1.00	12.21	6
ATOH	3868	CO2	TYR A 480	19.177	16.496	1.294	1.00	12.89	6
ATOH	3869	CZ	TYR A 480						
ATOH	3870	OIL	TYR A 480						
ATOH	3871	C	TYR A 480						
ATOH	3872	O	TYR A 480						
ATOH	3873	N	VAL A 481						
ATOH	3874	CA	VAL A 481						
ATOH	3875	CB	VAL A 481						
ATOH	3876	CG1	VAL A 481						
ATOH	3877	CG2	VAL A 481						
ATOH	3878	C	VAL A 481						
ATOH	3879	O	VAL A 481						
ATOH	3880	N	GLN A 482						
ATOH	3881	CA	GLN A 482						
ATOH	3882	CB	GLN A 482						
ATOH	3883	CG	GLN A 482						
ATOH	3884	CD	GLN A 482						
ATOH	3885	OE1	GLN A 482						
ATOH	3886	NE2	GLN A 482						
ATOH	3887	C	GLN A 482						
ATOH	3888	O	GLN A 482						
ATOH	3889	N	ARG A 483						
ATOH	3890	CA	ARG A 483						
ATOH	3891	CB	ARG A 483						
ATOH	3892	CG	ARG A 483						
ATOH	3893	CD	ARG A 483						
ATOH	3894	CE	ARG A 483						
ATOH	3895	CZ	ARG A 483						
ATOH	3896	NI1	ARG A 483						
ATOH	3897	NI2	ARG A 483						
ATOH	3898	C	ARG A 483						
ATOH	3899	O	ARG A 483						
ATOH	3900	OT	ARG A 483						
ATOH	3901	CA	IUH \$ 501						
ATOH	3902	CA	IUH \$ 502						
ATOH	3903	CA	IUH \$ 503						
ATOH	3904	CA	IUH \$ 504						
ATOH	3905	OM1	WAT X 1						
ATOH	3906	OM2	WAT X 1						
ATOH	3907	OM3	WAT X 1						
ATOH	3908	OM4	WAT X 1						
ATOH	3909	OM5	WAT X 1						
ATOH	3910	OM6	WAT X 1						
ATOH	3911	OM7	WAT X 1						
ATOH	3912	OM8	WAT X 1						
ATOH	3913	OM9	WAT X 1						
ATOH	3914	OM10	WAT X 2						
ATOH	3915	OM11	WAT X 2						
ATOH	3916	OM12	WAT X 2						
ATOH	3917	OM13	WAT X 2						
ATOH	3918	OM14	WAT X 2						
ATOH	3919	OM15	WAT X 2						
ATOH	3920	OM16	WAT X 2						
ATOH	3921	OM17	WAT X 2						
ATOH	3922	OM18	WAT X 2						

ATOM	3923	049	WAT	X	2	42.991	28.597	56.879	1.00	19.54	8	ATOM	3976	042	WAT	X	8	18.586	45.140	20.306	1.00	24.89	8
ATOM	3924	040	WAT	X	3	42.416	33.909	17.726	1.00	10.85	8	ATOM	3977	043	WAT	X	8	40.969	25.117	33.960	1.00	19.79	8
ATOM	3925	041	WAT	X	3	48.842	22.953	44.340	1.00	7.46	8	ATOM	3978	044	WAT	X	8	20.088	43.470	17.087	1.00	16.72	8
ATOM	3926	042	WAT	X	3	36.038	55.628	43.083	1.00	10.34	8	ATOM	3979	045	WAT	X	8	38.467	37.011	11.354	1.00	25.51	8
ATOM	3927	043	WAT	X	3	58.570	25.578	42.683	1.00	12.51	8	ATOM	3980	046	WAT	X	8	13.729	9.292	-1.198	1.00	18.29	8
ATOM	3928	044	WAT	X	3	35.732	43.524	49.882	1.00	5.95	8	ATOM	3981	047	WAT	X	8	37.082	34.587	46.550	1.00	20.44	8
ATOM	3929	045	WAT	X	3	26.190	18.692	1.154	1.00	12.57	8	ATOM	3982	048	WAT	X	8	33.674	26.739	26.941	1.00	37.20	8
ATOM	3930	046	WAT	X	3	40.723	25.525	46.044	1.00	10.44	8	ATOM	3983	049	WAT	X	8	44.040	39.609	29.378	1.00	15.09	8
ATOM	3931	047	WAT	X	3	36.546	42.416	33.352	1.00	5.00	8	ATOM	3984	040	WAT	X	9	5.980	17.940	10.956	1.00	15.78	8
ATOM	3932	048	WAT	X	3	40.987	21.110	52.091	1.00	20.54	8	ATOM	3985	041	WAT	X	9	37.928	39.774	25.743	1.00	20.89	8
ATOM	3933	049	WAT	X	4	37.695	27.410	12.493	1.00	11.34	8	ATOM	3986	042	WAT	X	9	30.894	54.048	35.873	1.00	15.39	8
ATOM	3934	040	WAT	X	4	22.844	23.707	36.872	1.00	9.80	8	ATOM	3987	043	WAT	X	9	28.071	34.048	54.110	1.00	17.12	8
ATOM	3935	041	WAT	X	4	36.012	18.648	48.284	1.00	17.35	8	ATOM	3988	044	WAT	X	9	18.742	28.715	32.238	1.00	16.32	8
ATOM	3936	042	WAT	X	4	31.899	45.870	33.523	1.00	10.56	8	ATOM	3989	045	WAT	X	9	21.957	31.164	51.343	1.00	17.53	8
ATOM	3937	043	WAT	X	4	30.501	38.096	33.954	1.00	11.67	8	ATOM	3990	046	WAT	X	9	17.533	31.407	37.350	1.00	18.05	8
ATOM	3938	044	WAT	X	4	22.073	12.907	32.231	1.00	10.97	8	ATOM	3991	047	WAT	X	9	33.329	26.312	6.343	1.00	16.49	8
ATOM	3939	045	WAT	X	4	40.488	14.451	42.396	1.00	12.74	8	ATOM	3992	048	WAT	X	9	33.954	32.866	59.563	1.00	22.51	8
ATOM	3940	046	WAT	X	4	53.405	37.236	44.839	1.00	12.00	8	ATOM	3993	049	WAT	X	9	20.209	19.419	22.073	1.00	15.65	8
ATOM	3941	047	WAT	X	4	43.396	20.817	52.968	1.00	25.21	8	ATOM	3994	040	WAT	X	10	32.236	16.522	47.616	1.00	20.65	8
ATOM	3942	048	WAT	X	4	45.712	34.753	17.330	1.00	22.47	8	ATOM	3995	041	WAT	X	10	29.512	27.238	32.842	1.00	17.87	8
ATOM	3943	049	WAT	X	4	52.299	25.204	54.738	1.00	18.85	8	ATOM	3996	042	WAT	X	10	38.117	21.774	-1.117	1.00	25.65	8
ATOM	3944	040	WAT	X	5	10.466	19.211	8.671	1.00	8.04	8	ATOM	3997	043	WAT	X	10	36.476	40.547	18.282	1.00	25.86	8
ATOM	3945	041	WAT	X	5	23.407	21.100	30.729	1.00	15.19	8	ATOM	3998	044	WAT	X	10	18.917	5.144	16.972	1.00	16.17	8
ATOM	3946	042	WAT	X	5	34.672	39.007	47.914	1.00	25.93	8	ATOM	3999	045	WAT	X	10	23.106	43.383	45.060	1.00	22.47	8
ATOM	3947	043	WAT	X	5	39.440	24.513	6.213	1.00	20.60	8	ATOM	4000	046	WAT	X	10	27.983	24.700	5.027	1.00	20.60	8
ATOM	3948	044	WAT	X	5	43.207	54.381	40.149	1.00	25.71	8	ATOM	4001	047	WAT	X	10	34.986	39.869	15.784	1.00	23.70	8
ATOM	3949	045	WAT	X	5	29.887	49.393	26.775	1.00	10.08	8	ATOM	4002	048	WAT	X	10	5.987	15.831	-1.902	1.00	32.41	8
ATOM	3950	046	WAT	X	5	18.296	28.320	27.646	1.00	17.61	8	ATOM	4003	049	WAT	X	10	19.643	16.427	-2.512	1.00	35.14	8
ATOM	3951	047	WAT	X	5	42.657	37.701	31.679	1.00	16.67	8	ATOM	4004	040	WAT	X	11	17.172	19.237	19.676	1.00	29.78	8
ATOM	3952	048	WAT	X	5	27.361	18.395	39.419	1.00	14.74	8	ATOM	4005	041	WAT	X	11	49.760	21.003	51.233	1.00	9.95	8
ATOM	3953	049	WAT	X	5	28.339	52.900	35.976	1.00	18.51	8	ATOM	4006	042	WAT	X	11	41.639	31.412	35.004	1.00	25.82	8
ATOM	3954	040	WAT	X	6	37.756	14.989	39.100	1.00	17.01	8	ATOM	4007	043	WAT	X	11	25.364	51.628	41.093	1.00	29.63	8
ATOM	3955	041	WAT	X	6	22.840	21.238	35.474	1.00	13.60	8	ATOM	4008	044	WAT	X	11	42.937	27.882	12.460	1.00	33.98	8
ATOM	3956	042	WAT	X	6	38.940	13.232	9.026	1.00	11.51	8	ATOM	4009	045	WAT	X	11	18.451	29.166	35.333	1.00	27.81	8
ATOM	3957	043	WAT	X	6	25.342	16.185	20.356	1.00	18.86	8	ATOM	4010	046	WAT	X	11	24.969	26.021	50.840	1.00	26.74	8
ATOM	3958	044	WAT	X	6	8.361	17.329	8.642	1.00	13.52	8	ATOM	4011	047	WAT	X	11	43.160	54.157	43.072	1.00	23.83	8
ATOM	3959	045	WAT	X	6	37.794	6.917	7.269	1.00	20.73	8	ATOM	4012	048	WAT	X	11	12.642	37.968	31.162	1.00	65.20	8
ATOM	3960	046	WAT	X	6	45.060	49.979	33.793	1.00	12.44	8	ATOM	4013	049	WAT	X	11	32.411	23.218	5.138	1.00	18.08	8
ATOM	3961	047	WAT	X	6	36.427	41.328	48.308	1.00	11.02	8	ATOM	4014	040	WAT	X	12	19.308	3.707	13.407	1.00	50.55	8
ATOM	3962	048	WAT	X	6	41.263	15.827	37.266	1.00	22.49	8	ATOM	4015	041	WAT	X	12	17.400	20.494	-1.396	1.00	25.22	8
ATOM	3963	049	WAT	X	6	25.131	39.394	49.866	1.00	10.30	8	ATOM	4016	042	WAT	X	12	38.504	40.778	36.668	1.00	40.52	8
ATOM	3964	040	WAT	X	7	51.050	21.873	54.397	1.00	18.11	8	ATOM	4017	043	WAT	X	12	46.693	16.740	48.249	1.00	22.77	8
ATOM	3965	041	WAT	X	7	48.952	26.479	52.035	1.00	17.95	8	ATOM	4018	044	WAT	X	12	29.593	23.052	4.777	1.00	30.69	8
ATOM	3966	042	WAT	X	7	24.717	49.514	27.044	1.00	19.57	8	ATOM	4019	045	WAT	X	12	25.325	25.894	6.415	1.00	23.43	8
ATOM	3967	043	WAT	X	7	32.551	52.703	28.488	1.00	9.04	8	ATOM	4020	046	WAT	X	12	37.028	10.496	27.680	1.00	13.65	8
ATOM	3968	044	WAT	X	7	44.885	26.009	54.445	1.00	7.24	8	ATOM	4021	047	WAT	X	12	15.428	33.267	21.245	1.00	27.08	8
ATOM	3969	045	WAT	X	7	38.325	36.644	45.393	1.00	19.65	8	ATOM	4022	048	WAT	X	12	32.665	39.080	54.672	1.00	21.60	8
ATOM	3970	046	WAT	X	7	21.609	12.965	20.907	1.00	9.32	8	ATOM	4023	049	WAT	X	13	46.251	40.891	31.602	1.00	25.79	8
ATOM	3971	047	WAT	X	7	24.711	13.545	20.784	1.00	23.06	8	ATOM	4024	040	WAT	X	13	38.486	30.224	30.783	1.00	20.87	8
ATOM	3972	048	WAT	X	7	42.374	43.789	25.824	1.00	28.85	8	ATOM	4025	041	WAT	X	13	42.551	46.583	21.900	1.00	28.42	8
ATOM	3973	049	WAT	X	7							ATOM	4026	042	WAT	X	13						
ATOM	3974	040	WAT	X	8							ATOM	4027	043	WAT	X	13						
ATOM	3975	041	WAT	X	8							ATOM	4028	044	WAT	X	13						

ATOM	4029	OH5	WAT	X	13	13.009	12.182	-4.047	1.00	27.61	8
ATOM	4030	OH6	WAT	X	13	32.756	8.582	1.824	1.00	29.04	8
ATOM	4031	OH7	WAT	X	13	16.249	23.415	-2.919	1.00	36.05	8
ATOM	4032	OH8	WAT	X	13	36.916	46.802	51.068	1.00	13.92	8
ATOM	4033	OH9	WAT	X	13	51.456	45.867	53.043	1.00	27.25	8
ATOM	4034	OH0	WAT	X	14	44.576	23.979	15.915	1.00	39.18	8
ATOM	4035	OH1	WAT	X	14	16.344	4.264	16.031	1.00	22.00	8
ATOM	4036	OH2	WAT	X	14	32.347	13.546	-3.049	1.00	37.27	8
ATOM	4037	OH3	WAT	X	14	45.366	38.058	33.758	1.00	20.90	8
ATOM	4038	OH4	WAT	X	14	4.549	18.600	13.099	1.00	20.30	8
ATOM	4039	OH5	WAT	X	14	15.354	36.796	43.569	1.00	18.79	8
ATOM	4040	OH6	WAT	X	14	44.963	30.462	57.791	1.00	33.45	8
ATOM	4041	OH7	WAT	X	14	53.136	23.195	37.475	1.00	31.43	8
ATOM	4042	OH8	WAT	X	14	30.694	15.659	-3.842	1.00	23.59	8
ATOM	4043	OH9	WAT	X	14	39.010	7.257	14.525	1.00	37.98	8
ATOM	4044	OH0	WAT	X	15	37.498	55.360	32.899	1.00	35.04	8
ATOM	4045	OH1	WAT	X	15	21.133	44.448	35.481	1.00	35.84	8
ATOM	4046	OH2	WAT	X	15	23.993	4.153	14.519	1.00	20.07	8
ATOM	4047	OH3	WAT	X	15	21.568	23.231	44.662	1.00	34.60	8
ATOM	4048	OH4	WAT	X	15	9.185	24.466	6.708	1.00	19.79	8
ATOM	4049	OH5	WAT	X	15	44.586	35.812	31.349	1.00	48.30	8
ATOM	4050	OH6	WAT	X	15	30.709	25.745	52.371	1.00	38.63	8
ATOM	4051	OH7	WAT	X	15	41.284	38.972	11.403	1.00	29.22	8
ATOM	4052	OH8	WAT	X	15	56.979	36.187	58.016	1.00	37.19	8
ATOM	4053	OH9	WAT	X	15	25.886	5.827	3.524	1.00	21.64	8
ATOM	4054	OH0	WAT	X	16	41.689	14.341	39.346	1.00	28.91	8
ATOM	4055	OH1	WAT	X	16	20.238	10.905	31.899	1.00	29.69	8
ATOM	4056	OH2	WAT	X	16	44.542	44.756	52.978	1.00	18.83	8
ATOM	4057	OH3	WAT	X	16	57.377	17.228	51.604	1.00	20.62	8
ATOM	4058	OH4	WAT	X	16	53.851	33.580	56.957	1.00	22.46	8
ATOM	4059	OH5	WAT	X	16	35.776	25.007	52.963	1.00	30.96	8
ATOM	4060	OH6	WAT	X	16	50.697	26.378	37.894	1.00	17.69	8
ATOM	4061	OH7	WAT	X	16	35.244	16.237	47.346	1.00	35.92	8
ATOM	4062	OH8	WAT	X	16	41.297	31.972	30.043	1.00	23.15	8
ATOM	4063	OH9	WAT	X	16	60.104	21.780	53.887	1.00	24.69	8
ATOM	4064	OH0	WAT	X	17	33.930	36.911	56.317	1.00	28.54	8
ATOM	4065	OH1	WAT	X	17	27.783	49.620	50.985	1.00	21.73	8
ATOM	4066	OH2	WAT	X	17	38.322	12.309	23.483	1.00	42.93	8
ATOM	4067	OH3	WAT	X	17	19.759	16.587	26.896	1.00	25.91	8
ATOM	4068	OH4	WAT	X	17	18.392	24.561	-0.866	1.00	45.44	8
ATOM	4069	OH5	WAT	X	17	43.370	16.553	29.268	1.00	24.28	8
ATOM	4070	OH6	WAT	X	17	12.508	25.520	4.810	1.00	39.21	8
ATOM	4071	OH7	WAT	X	17	44.009	35.484	9.586	1.00	24.72	8
ATOM	4072	OH8	WAT	X	17	38.155	15.958	4.049	1.00	27.73	8
ATOM	4073	OH9	WAT	X	17	32.659	22.367	51.695	1.00	36.96	8
ATOM	4074	OH0	WAT	X	18	8.655	11.822	18.551	1.00	22.83	8
ATOM	4075	OH1	WAT	X	18	61.442	16.332	49.671	1.00	35.09	8
ATOM	4076	OH2	WAT	X	18	52.691	20.468	49.830	1.00	27.27	8
ATOM	4077	OH3	WAT	X	18	33.981	29.452	4.620	1.00	46.70	8
ATOM	4078	OH4	WAT	X	18	22.398	9.094	32.744	1.00	31.90	8
ATOM	4079	OH5	WAT	X	18	24.654	27.519	4.442	1.00	26.37	8
ATOM	4080	OH6	WAT	X	18	24.112	52.226	27.595	1.00	38.43	8
ATOM	4081	OH7	WAT	X	18	33.663	55.271	29.435	1.00	43.20	8
ATOM	4082	OH8	WAT	X	18	30.748	53.658	50.670	1.00	29.38	8
ATOM	4083	OH9	WAT	X	18	50.065	24.808	35.502	1.00	35.76	8
ATOM	4084	OH0	WAT	X	19	22.202	19.032	28.774	1.00	27.27	8
ATOM	4085	OH1	WAT	X	19	54.614	46.941	48.285	1.00	29.46	8
ATOM	4086	OH2	WAT	X	19	46.049	21.147	25.386	1.00	33.35	8
ATOM	4087	OH3	WAT	X	19	45.816	49.038	43.196	1.00	33.55	8
ATOM	4088	OH4	WAT	X	19	22.659	43.614	47.560	1.00	46.32	8
ATOM	4089	OH5	WAT	X	19	60.822	30.153	59.870	1.00	43.42	8
ATOM	4090	OH6	WAT	X	19	53.393	13.840	38.545	1.00	36.26	8
ATOM	4091	OH7	WAT	X	19	32.544	1.677	6.989	1.00	38.69	8
ATOM	4092	OH8	WAT	X	19	50.647	31.408	63.808	1.00	33.78	8
ATOM	4093	OH9	WAT	X	19	16.948	27.505	19.812	1.00	23.95	8
ATOM	4094	OH0	WAT	X	20	6.330	5.129	-1.860	1.00	55.10	8
ATOM	4095	OH1	WAT	X	20	32.149	29.484	1.396	1.00	29.24	8
ATOM	4096	OH2	WAT	X	20	18.952	20.628	24.894	1.00	35.86	8
ATOM	4097	OH3	WAT	X	20	31.733	56.172	34.803	1.00	38.99	8
ATOM	4098	OH4	WAT	X	20	54.293	14.452	50.415	1.00	35.67	8
ATOM	4099	OH5	WAT	X	20	44.169	20.632	26.756	1.00	27.57	8
ATOM	4100	OH6	WAT	X	20	25.114	53.998	30.655	1.00	43.33	8
ATOM	4101	OH7	WAT	X	20	43.966	46.309	55.136	1.00	37.54	8
ATOM	4102	OH8	WAT	X	20	58.366	45.019	48.175	1.00	43.14	8
ATOM	4103	OH9	WAT	X	20	44.205	21.201	13.125	1.00	51.53	8
ATOM	4104	OH0	WAT	X	21	61.128	25.016	42.919	1.00	34.86	8
ATOM	4105	OH1	WAT	X	21	8.371	24.444	12.113	1.00	45.95	8
ATOM	4106	OH2	WAT	X	21	18.370	31.505	12.739	1.00	27.20	8
ATOM	4107	OH3	WAT	X	21	33.430	25.045	51.739	1.00	31.92	8
ATOM	4108	OH4	WAT	X	21	47.660	31.418	59.018	1.00	35.64	8
ATOM	4109	OH5	WAT	X	21	43.308	25.115	12.609	1.00	40.37	8
ATOM	4110	OH6	WAT	X	21	44.725	50.787	28.523	1.00	26.83	8
ATOM	4111	OH7	WAT	X	21	40.073	41.591	56.477	1.00	38.23	8
ATOM	4112	OH8	WAT	X	21	3.706	15.718	9.641	1.00	23.55	8
ATOM	4113	OH9	WAT	X	21	46.527	18.879	50.827	1.00	35.55	8
ATOM	4114	OH0	WAT	X	22	51.052	12.865	45.163	1.00	48.72	8
ATOM	4115	OH1	WAT	X	22	54.191	42.505	55.913	1.00	22.39	8
ATOM	4116	OH2	WAT	X	22	65.480	31.263	47.436	1.00	36.62	8
ATOM	4117	OH3	WAT	X	22	30.283	47.935	54.169	1.00	31.71	8
ATOM	4118	OH4	WAT	X	22	35.283	36.318	46.899	1.00	68.71	8
ATOM	4119	OH5	WAT	X	22	47.871	46.056	38.969	1.00	32.78	8
ATOM	4120	OH6	WAT	X	22	37.896	8.826	3.495	1.00	35.54	8
ATOM	4121	OH7	WAT	X	22	35.101	8.628	38.130	1.00	35.44	8
ATOM	4122	OH8	WAT	X	22	38.308	4.945	9.263	1.00	39.44	8
ATOM	4123	OH9	WAT	X	22	29.192	42.186	18.601	1.00	42.65	8
ATOM	4124	OH0	WAT	X	23	43.449	25.207	33.605	1.00	44.04	8
ATOM	4125	OH1	WAT	X	23	42.056	26.583	57.914	1.00	29.94	8
ATOM	4126	OH2	WAT	X	23	15.436	32.096	27.975	1.00	37.43	8
ATOM	4127	OH3	WAT	X	23	40.123	43.268	18.152	1.00	32.32	8
ATOM	4128	OH4	WAT	X	23	14.301	18.529	21.331	1.00	42.06	8
ATOM	4129	OH5	WAT	X	23	41.316	39.786	58.213	1.00	39.62	8
ATOM	4130	OH6	WAT	X	23	28.167	15.941	46.987	1.00	33.05	8
ATOM	4131	OH7	WAT	X	23	62.463	32.861	38.118	1.00	24.23	8
ATOM	4132	OH8	WAT	X	23	50.420	44.042	41.952	1.00	37.32	8
ATOM	4133	OH9	WAT	X	23	30.486	6.686	18.716	1.00	38.40	8
ATOM	4134	OH0	WAT	X	24	39.000	11.315	44.273	1.00	38.40	8

4135	ATOM	0415	WAT	X	24	26.342	44.862	18.030	1.00	27.39	8
4136	ATOM	042	WAT	X	24	42.233	42.967	22.516	1.00	28.16	8
4137	ATOM	043	WAT	X	24	17.859	41.857	40.950	1.00	44.87	8
4138	ATOM	044	WAT	X	24	18.774	45.302	34.094	1.00	36.85	8
4139	ATOM	045	WAT	X	24	17.379	48.385	29.218	1.00	36.40	8
4140	ATOM	046	WAT	X	24	59.859	17.628	38.947	1.00	24.00	8
4141	ATOM	047	WAT	X	24	44.716	26.845	15.361	1.00	31.66	8
4142	ATOM	048	WAT	X	24	16.851	22.367	25.144	1.00	38.33	8
4143	ATOM	049	WAT	X	24	44.428	18.344	31.454	1.00	28.87	8
4144	ATOM	050	WAT	X	25	53.824	36.690	57.769	1.00	27.33	8
4145	ATOM	051	WAT	X	25	53.688	40.328	57.339	1.00	34.91	8
4146	ATOM	052	WAT	X	25	46.373	15.118	12.832	1.00	38.80	8
4147	ATOM	053	WAT	X	25	29.409	35.711	7.581	1.00	30.09	8
4148	ATOM	054	WAT	X	25	26.515	13.237	-3.213	1.00	30.52	8
4149	ATOM	055	WAT	X	25	20.273	3.147	6.130	1.00	29.22	8
4150	ATOM	056	WAT	X	25	34.514	42.011	19.633	1.00	23.60	8
4151	ATOM	057	WAT	X	25	41.463	52.238	24.622	1.00	33.83	8
4152	ATOM	058	WAT	X	25	18.346	37.804	42.302	1.00	35.93	8
4153	ATOM	059	WAT	X	25	35.262	54.671	32.179	1.00	58.94	8
4154	ATOM	060	WAT	X	26	44.229	16.673	16.585	1.00	37.25	8
4155	ATOM	061	WAT	X	26	44.766	14.121	14.699	1.00	46.53	8
4156	ATOM	062	WAT	X	26	31.390	33.920	59.134	1.00	33.03	8
4157	ATOM	063	WAT	X	26	12.971	21.397	23.449	1.00	37.99	8
4158	ATOM	064	WAT	X	26	41.259	51.310	51.509	1.00	40.81	8
4159	ATOM	065	WAT	X	26	41.929	11.622	42.697	1.00	45.17	8
4160	ATOM	066	WAT	X	26	42.707	44.751	57.570	1.00	42.32	8
4161	ATOM	067	WAT	X	26	56.463	13.749	51.681	1.00	36.66	8
4162	ATOM	068	WAT	X	26	24.821	43.342	-3.728	1.00	33.27	8
4163	ATOM	069	WAT	X	26	60.493	39.175	53.713	1.00	47.98	8
4164	ATOM	070	WAT	X	27	45.625	38.306	11.910	1.00	37.28	8
4165	ATOM	071	WAT	X	27	43.801	49.874	24.898	1.00	75.50	8
4166	ATOM	072	WAT	X	27	11.684	17.068	21.179	1.00	34.01	8
4167	ATOM	073	WAT	X	27	28.216	2.149	14.807	1.00	42.07	8
4168	ATOM	074	WAT	X	27	52.604	30.867	37.880	1.00	33.10	8
4169	ATOM	075	WAT	X	27	55.458	34.651	38.180	1.00	47.45	8
4170	ATOM	076	WAT	X	27	49.808	19.847	34.189	1.00	33.89	8
4171	ATOM	077	WAT	X	27	1.703	6.632	4.199	1.00	62.88	8
4172	ATOM	078	WAT	X	27	48.275	39.555	43.586	1.00	28.38	8
4173	ATOM	079	WAT	X	27	23.075	20.226	-6.003	1.00	61.62	8
4174	ATOM	080	WAT	X	28	38.679	43.247	57.111	1.00	53.07	8
4175	ATOM	081	WAT	X	28	21.533	51.639	33.545	1.00	49.86	8
4176	ATOM	082	WAT	X	28	1.544	11.851	5.024	1.00	69.29	8
4177	ATOM	083	WAT	X	28	22.566	43.229	15.525	1.00	28.33	8
4178	ATOM	084	WAT	X	28	44.851	57.241	34.859	1.00	42.49	8
4179	ATOM	085	WAT	X	28	33.378	9.541	42.581	1.00	51.22	8
4180	ATOM	086	WAT	X	28	27.186	6.024	-0.021	1.00	46.35	8
4181	ATOM	087	WAT	X	28	56.162	41.254	59.120	1.00	56.59	8
4182	ATOM	088	WAT	X	28	5.756	19.201	7.132	1.00	20.05	8
4183	ATOM	089	WAT	X	28	14.700	29.886	48.605	1.00	35.67	8
4184	ATOM	090	WAT	X	29	41.585	56.275	32.373	1.00	40.13	8
4185	ATOM	091	WAT	X	29	24.084	49.694	43.922	1.00	42.12	8
4186	ATOM	092	WAT	X	29	29.979	22.421	2.045	1.00	42.88	8
4187	ATOM	093	WAT	X	29	18.885	13.752	26.566	1.00	49.31	8
4188	ATOM	04188	WAT	X	29	33.246	35.860	58.555	1.00	24.66	8
4189	ATOM	04189	WAT	X	29	20.518	10.712	22.033	1.00	31.01	8
4190	ATOM	04190	WAT	X	29	28.355	41.870	50.614	1.00	38.09	8
4191	ATOM	04191	WAT	X	29	51.144	33.741	38.200	1.00	28.11	8
4192	ATOM	04192	WAT	X	29	50.909	32.604	61.158	1.00	44.30	8
4193	ATOM	04193	WAT	X	29	45.397	9.987	33.816	1.00	41.23	8
4194	ATOM	04194	WAT	X	30	45.383	21.851	32.647	1.00	34.24	8
4195	ATOM	04195	WAT	X	30	51.981	22.543	34.910	1.00	43.50	8
4196	ATOM	04196	WAT	X	30	35.294	58.821	39.452	1.00	34.28	8
4197	ATOM	04197	WAT	X	30	34.193	44.616	18.067	1.00	42.78	8
4198	ATOM	04198	WAT	X	30	31.695	52.889	53.190	1.00	54.83	8
4199	ATOM	04199	WAT	X	30	13.657	44.210	31.115	1.00	42.94	8
4200	ATOM	04200	WAT	X	30	17.493	40.635	13.227	1.00	54.30	8
4201	ATOM	04201	WAT	X	30	24.521	11.373	22.566	1.00	42.89	8
4202	ATOM	04202	WAT	X	30	37.671	38.607	58.700	1.00	67.82	8
4203	ATOM	04203	WAT	X	30	8.539	26.332	10.421	1.00	56.80	8
4204	ATOM	04204	WAT	X	31	49.681	16.792	34.456	1.00	56.81	8
4205	ATOM	04205	WAT	X	31	7.284	6.777	13.925	1.00	41.62	8
4206	ATOM	04206	WAT	X	31	19.842	44.869	37.796	1.00	32.48	8
4207	ATOM	04207	WAT	X	31	16.806	43.159	34.050	1.00	31.63	8
4208	ATOM	04208	WAT	X	31	40.080	55.247	29.931	1.00	46.41	8
4209	ATOM	04209	WAT	X	31	4.298	25.496	15.931	1.00	55.22	8
4210	ATOM	04210	WAT	X	31	49.649	40.424	40.847	1.00	31.66	8
4211	ATOM	04211	WAT	X	31	22.128	29.127	52.419	1.00	40.80	8
4212	ATOM	04212	WAT	X	31	16.243	33.605	36.184	1.00	38.09	8
4213	ATOM	04213	WAT	X	31	27.033	55.215	28.323	1.00	31.92	8
4214	ATOM	04214	WAT	X	32	16.931	37.637	36.501	1.00	32.22	8
4215	ATOM	04215	WAT	X	32	7.050	10.385	16.890	1.00	37.40	8
4216	ATOM	04216	WAT	X	32	50.382	29.410	35.312	1.00	56.52	8
4217	ATOM	04217	WAT	X	32	27.086	47.626	17.616	1.00	31.50	8
4218	ATOM	04218	WAT	X	32	50.029	47.652	42.125	1.00	45.87	8
4219	ATOM	04219	WAT	X	32	29.154	55.495	24.292	1.00	53.90	8
4220	ATOM	04220	WAT	X	32	32.970	58.606	36.552	1.00	46.22	8
4221	ATOM	04221	WAT	X	32	43.201	24.152	56.971	1.00	59.17	8
4222	ATOM	04222	WAT	X	32	41.947	30.732	9.284	1.00	45.99	8
4223	ATOM	04223	WAT	X	32	21.381	14.261	36.815	1.00	44.69	8
4224	ATOM	04224	WAT	X	33	60.941	22.089	43.042	1.00	37.06	8
4225	ATOM	04225	WAT	X	33	40.505	56.155	42.947	1.00	68.99	8
4226	ATOM	04226	WAT	X	33	18.578	37.434	47.553	1.00	35.06	8
4227	ATOM	04227	WAT	X	33	31.707	48.490	18.182	1.00	32.40	8
4228	ATOM	04228	WAT	X	33	20.611	21.237	38.626	1.00	41.44	8
4229	ATOM	04229	WAT	X	33	38.037	8.708	21.690	1.00	53.54	8
4230	ATOM	04230	WAT	X	33	18.925	37.694	11.766	1.00	57.07	8
4231	ATOM	04231	WAT	X	33	53.097	28.032	37.987	1.00	57.12	8
4232	ATOM	04232	WAT	X	33	63.148	36.349	37.733	1.00	40.38	8
4233	ATOM	04233	WAT	X	34	14.116	36.171	21.843	1.00	42.46	8
4234	ATOM	04234	WAT	X	34	22.608	32.412	5.553	1.00	37.92	8
4235	ATOM	04235	WAT	X	34	29.443	3.779	16.367	1.00	46.74	8
4236	ATOM	04236	WAT	X	34	41.862	17.565	7.880	1.00	10.16	8
4237	ATOM	04237	WAT	X	34	44.558	18.412	8.333	1.00	38.61	8
4238	ATOM	04238	WAT	X	34	51.913	26.058	58.542	1.00	43.05	8
4239	ATOM	04239	WAT	X	34	64.063	33.656	56.634	1.00	55.33	8
4240	ATOM	04240	WAT	X	34	34.660	53.702	52.276	1.00	47.20	8

4241	ATOH	0408	WAT	X	34	5.844	14.713	12.911	1.00	40.12	8
4242	ATOH	0409	WAT	X	34	39.697	54.257	50.395	1.00	36.68	8
4243	ATOH	0410	WAT	X	35	18.706	24.537	40.234	1.00	51.89	8
4244	ATOH	0411	WAT	X	35	20.209	21.570	34.426	1.00	34.23	8
4245	ATOH	0412	WAT	X	35	44.584	17.646	26.801	1.00	35.45	8
4246	ATOH	0413	WAT	X	35	61.438	32.246	57.799	1.00	36.05	8
4247	ATOH	0414	WAT	X	35	13.266	6.166	0.033	1.00	49.60	8
4248	ATOH	0415	WAT	X	35	42.142	53.175	26.887	1.00	43.15	8
4249	ATOH	0416	WAT	X	35	33.505	54.214	55.522	1.00	56.63	8
4250	ATOH	0417	WAT	X	35	1.397	8.422	6.873	1.00	48.68	8
4251	ATOH	0418	WAT	X	35	47.778	11.907	38.953	1.00	34.48	8
4252	ATOH	0419	WAT	X	35	15.856	27.767	43.603	1.00	55.40	8
4253	ATOH	0420	WAT	X	36	38.734	7.626	16.829	1.00	43.46	8
4254	ATOH	0421	WAT	X	36	10.578	1.626	2.281	1.00	40.52	8
4255	ATOH	0422	WAT	X	36	50.000	33.901	35.051	1.00	49.14	8
4256	ATOH	0423	WAT	X	36	44.622	34.879	33.356	1.00	60.84	8
4257	ATOH	0424	WAT	X	36	3.016	16.327	21.655	1.00	60.04	8
4258	ATOH	0425	WAT	X	36	41.431	56.503	45.767	1.00	56.22	8
4259	ATOH	0426	WAT	X	36	49.548	26.337	22.216	1.00	53.09	8
4260	ATOH	0427	WAT	X	36	37.549	29.346	4.956	1.00	52.92	8
4261	ATOH	0428	WAT	X	36	49.260	44.486	55.149	1.00	38.00	8
4262	ATOH	0429	WAT	X	36	53.734	18.532	52.401	1.00	51.95	8
4263	ATOH	0430	WAT	X	37	39.061	11.166	25.898	1.00	36.59	8
4264	ATOH	0431	WAT	X	37	10.532	4.916	16.271	1.00	58.74	8
4265	ATOH	0432	WAT	X	37	41.366	7.373	32.768	1.00	44.27	8
4266	ATOH	0433	WAT	X	37	32.474	41.914	15.484	1.00	41.36	8
4267	ATOH	0434	WAT	X	37	18.592	28.534	17.648	1.00	40.22	8
4268	ATOH	0435	WAT	X	37	58.677	25.814	40.128	1.00	45.33	8
4269	ATOH	0436	WAT	X	37	15.567	6.537	19.083	1.00	49.88	8
4270	ATOH	0437	WAT	X	37	37.675	57.053	47.412	1.00	39.96	8
4271	ATOH	0438	WAT	X	37	49.434	37.594	42.185	1.00	42.38	8
4272	ATOH	0439	WAT	X	37	42.690	28.862	30.545	1.00	48.41	8
4273	ATOH	0440	WAT	X	38	29.822	6.331	24.708	1.00	36.08	8
4274	ATOH	0441	WAT	X	38	43.869	32.981	31.239	1.00	43.26	8
4275	ATOH	0442	WAT	X	38	16.119	10.852	-3.221	1.00	54.04	8
4276	ATOH	0443	WAT	X	38	46.051	14.381	33.005	1.00	58.57	8
4277	ATOH	0444	WAT	X	38	26.231	44.941	50.291	1.00	50.76	8
4278	ATOH	0445	WAT	X	38	41.500	26.375	9.990	1.00	49.03	8
4279	ATOH	0446	WAT	X	38	51.550	42.087	41.209	1.00	52.61	8
4280	ATOH	0447	WAT	X	38	38.215	7.892	30.920	1.00	43.87	8
4281	ATOH	0448	WAT	X	38	22.207	33.878	7.842	1.00	47.74	8
4282	ATOH	0449	WAT	X	39	49.722	41.667	12.969	1.00	59.07	8
4283	ATOH	0450	WAT	X	39	35.909	18.255	51.330	1.00	53.37	8
4284	ATOH	0451	WAT	X	39	43.924	10.373	31.316	1.00	42.79	8
4285	ATOH	0452	WAT	X	39	22.583	10.397	39.495	1.00	68.43	8
4286	ATOH	0453	WAT	X	39	19.514	48.906	21.847	1.00	66.89	8
4287	ATOH	0454	WAT	X	39	13.468	27.723	5.713	1.00	44.03	8
4288	ATOH	0455	WAT	X	39	45.654	25.542	63.943	1.00	37.57	8
4289	ATOH	0456	WAT	X	39	44.078	13.029	36.046	1.00	48.13	8
4290	ATOH	0457	WAT	X	39	27.240	0.087	12.290	1.00	45.09	8
4291	ATOH	0458	WAT	X	39	15.804	17.374	23.289	1.00	58.48	8
4292	ATOH	0459	WAT	X	40	23.294	12.036	34.534	1.00	60.75	8
4293	ATOH	0460	WAT	X	40	47.490	44.003	18.065	1.00	45.23	8
4294	ATOH	0461	WAT	X	40	17.196	19.679	22.860	1.00	53.81	8
4295	ATOH	0462	WAT	X	40	22.069	3.918	3.047	1.00	55.02	8
4296	ATOH	0463	WAT	X	40	40.725	28.659	11.393	1.00	42.24	8
4297	ATOH	0464	WAT	X	40	53.521	31.821	60.008	1.00	46.58	8
4298	ATOH	0465	WAT	X	40	43.778	45.011	23.792	1.00	52.91	8
4299	ATOH	0466	WAT	X	40	45.725	48.904	30.294	1.00	35.75	8
4300	ATOH	0467	WAT	X	40	49.126	11.559	46.679	1.00	49.02	8
4301	ATOH	0468	WAT	X	40	68.137	39.801	42.467	1.00	64.82	8
4302	ATOH	0469	WAT	X	40	19.785	19.132	28.386	1.00	38.16	8
4303	ATOH	0470	WAT	X	41	46.799	34.048	27.779	1.00	53.88	8
4304	ATOH	0471	WAT	X	41	46.195	38.407	29.718	1.00	67.17	8
4305	ATOH	0472	WAT	X	41	10.791	46.608	27.796	1.00	38.46	8
4306	ATOH	0473	WAT	X	41	17.255	25.962	28.182	1.00	49.71	8
4307	ATOH	0474	WAT	X	41	38.815	10.903	18.927	1.00	49.73	8
4308	ATOH	0475	WAT	X	41	47.017	51.069	47.161	1.00	58.10	8
4309	ATOH	0476	WAT	X	41	52.558	36.860	39.163	1.00	53.80	8
4310	ATOH	0477	WAT	X	41	19.024	23.922	31.261	1.00	60.30	8
4311	ATOH	0478	WAT	X	41	15.798	27.427	30.407	1.00	100.00	8
4312	ATOH	0479	WAT	X	42	55.428	38.709	38.776	1.00	50.63	8
4313	ATOH	0480	WAT	X	42	23.391	20.916	45.890	1.00	44.61	8
4314	ATOH	0481	WAT	X	42	4.072	14.391	18.394	1.00	42.40	8
4315	ATOH	0482	WAT	X	42	42.371	37.835	9.565	1.00	46.80	8
4316	ATOH	0483	WAT	X	42	6.020	13.143	15.676	1.00	60.89	8
4317	ATOH	0484	WAT	X	42	2.445	17.737	5.335	1.00	44.54	8
4318	ATOH	0485	WAT	X	42	39.431	8.272	34.812	1.00	46.23	8
4319	ATOH	0486	WAT	X	42	43.239	42.762	20.441	1.00	42.07	8
4320	ATOH	0487	WAT	X	42	43.667	29.029	33.074	1.00	53.81	8
4321	ATOH	0488	WAT	X	42	15.819	3.536	11.715	1.00	45.41	8
4322	ATOH	0489	WAT	X	43	22.756	6.724	-4.904	1.00	44.46	8
4323	ATOH	0490	WAT	X	43	32.918	47.694	61.485	1.00	67.38	8
4324	ATOH	0491	WAT	X	43	32.074	40.098	11.945	1.00	34.37	8
4325	ATOH	0492	WAT	X	43	44.790	41.553	18.449	1.00	44.94	8
4326	ATOH	0493	WAT	X	43	15.058	29.090	20.720	1.00	49.25	8
4327	ATOH	0494	WAT	X	43	24.069	18.351	48.150	1.00	62.06	8
4328	ATOH	0495	WAT	X	43	40.835	26.920	30.843	1.00	49.68	8
4329	ATOH	0496	WAT	X	43	7.082	2.097	8.379	1.00	47.50	8
4330	ATOH	0497	WAT	X	43	47.039	51.990	40.775	1.00	51.23	8
4331	ATOH	0498	WAT	X	43	22.252	13.968	43.293	1.00	38.13	8
4332	ATOH	0499	WAT	X	44	25.106	31.488	52.711	1.00	57.06	8
4333	ATOH	0500	WAT	X	44	23.054	7.691	28.407	1.00	52.15	8
4334	ATOH	0501	WAT	X	44	21.526	1.631	11.156	1.00	53.95	8
4335	ATOH	0502	WAT	X	44	20.140	16.123	39.073	1.00	62.86	8
4336	ATOH	0503	WAT	X	44	17.491	51.997	31.031	1.00	80.00	8
4337	ATOH	0504	WAT	X	44	46.380	42.021	59.675	1.00	51.50	8
4338	ATOH	0505	WAT	X	44	13.481	34.188	29.544	1.00	66.53	8
4339	ATOH	0506	WAT	X	44	33.452	41.508	56.803	1.00	50.62	8
4340	ATOH	0507	WAT	X	44	47.624	43.632	31.945	1.00	43.18	8
4341	ATOH	0508	WAT	X	44	26.231	12.181	43.880	1.00	49.95	8
4342	ATOH	0509	WAT	X	45	14.968	36.024	33.676	1.00	63.17	8
4343	ATOH	0510	WAT	X	45	62.906	20.054	42.528	1.00	50.37	8
4344	ATOH	0511	WAT	X	45	45.852	21.374	58.053	1.00	55.98	8
4345	ATOH	0512	WAT	X	45	50.504	43.538	16.798	1.00	34.36	8
4346	ATOH	0513	WAT	X	45	36.077	40.800	13.082	1.00	45.23	8

ATOM	4347	OH5	WAT	X	45	15.297	36.178	30.314	1.00	41.94	8
ATOM	4348	OH6	WAT	X	45	11.948	34.622	19.560	1.00	83.16	8
ATOM	4349	OH8	WAT	X	45	49.746	24.887	60.391	1.00	66.28	8
ATOM	4350	OH9	WAT	X	45	36.657	55.115	28.131	1.00	37.69	8
ATOM	4351	OH0	WAT	X	46	55.074	25.248	36.950	1.00	41.36	8
ATOM	4352	OH1	WAT	X	46	47.652	23.423	22.484	1.00	42.59	8
ATOM	4353	OH2	WAT	X	46	44.015	15.772	24.447	1.00	47.57	8
ATOM	4354	OH3	WAT	X	46	7.635	2.279	10.856	1.00	61.51	8
ATOM	4355	OH4	WAT	X	46	55.490	45.238	53.756	1.00	80.18	8
ATOM	4356	OH5	WAT	X	46	24.651	30.369	3.824	1.00	53.51	8
ATOM	4357	OH6	WAT	X	46	36.564	25.795	58.795	1.00	43.24	8
ATOM	4358	OH7	WAT	X	46	37.878	24.510	56.673	1.00	60.23	8
ATOM	4359	OH8	WAT	X	46	9.767	27.253	17.228	1.00	44.01	8
ATOM	4360	OH9	WAT	X	46	33.066	7.229	37.529	1.00	48.47	8
ATOM	4361	OH0	WAT	X	47	8.243	21.706	21.929	1.00	61.56	8
ATOM	4362	OH1	WAT	X	47	46.978	13.274	45.175	1.00	40.90	8
ATOM	4363	OH2	WAT	X	47	41.004	12.753	21.561	1.00	73.88	8
ATOM	4364	OH3	WAT	X	47	3.035	8.918	-0.355	1.00	50.88	8
ATOM	4365	OH4	WAT	X	47	18.537	34.248	10.555	1.00	79.91	8
ATOM	4366	OH5	WAT	X	47	26.233	6.791	-2.079	1.00	48.58	8
ATOM	4367	OH6	WAT	X	47	37.312	53.735	22.566	1.00	63.31	8
ATOM	4368	OH7	WAT	X	47	17.940	29.638	6.277	1.00	57.32	8
ATOM	4369	OH8	WAT	X	47	26.830	27.316	2.717	1.00	62.15	8
ATOM	4370	OH9	WAT	X	47	65.931	28.577	46.176	1.00	69.51	8
ATOM	4371	OH0	WAT	X	48	19.661	45.120	40.540	1.00	40.74	8
ATOM	4372	OH1	WAT	X	48	10.667	22.744	23.628	1.00	36.22	8
ATOM	4373	OH2	WAT	X	48	8.702	24.434	20.838	1.00	51.66	8
ATOM	4374	OH3	WAT	X	48	35.773	26.533	56.343	1.00	38.96	8
ATOM	4375	OH4	WAT	X	48	38.218	2.333	13.072	1.00	37.60	8
ATOM	4376	OH5	WAT	X	48	25.061	48.128	50.748	1.00	69.43	8
ATOM	4377	OH6	WAT	X	48	24.333	37.538	52.402	1.00	33.69	8
ATOM	4378	OH7	WAT	X	48	52.741	13.029	46.552	1.00	46.94	8
ATOM	4379	OH8	WAT	X	48	30.393	18.085	52.715	1.00	73.77	8
ATOM	4380	OH9	WAT	X	49	21.293	35.987	52.496	1.00	56.71	8
ATOM	4381	OH0	WAT	X	49	26.704	53.743	20.826	1.00	82.73	8
ATOM	4382	OH1	WAT	X	49	65.451	38.921	50.670	1.00	50.91	8
ATOM	4383	OH2	WAT	X	49	9.019	18.103	21.967	1.00	57.54	8
ATOM	4384	OH3	WAT	X	49	43.689	31.759	26.580	1.00	33.20	8
ATOM	4385	OH4	WAT	X	49	65.973	31.154	38.950	1.00	51.21	8
ATOM	4386	OH5	WAT	X	49	50.668	41.968	57.102	1.00	65.20	8
ATOM	4387	OH6	WAT	X	49	67.466	32.818	48.733	1.00	35.55	8
ATOM	4388	OH7	WAT	X	49	12.540	31.451	14.136	1.00	67.07	8
ATOM	4389	OH8	WAT	X	49	24.089	6.493	18.874	1.00	41.89	8
ATOM	4390	OH9	WAT	X	50	46.352	12.360	48.271	1.00	78.91	8
ATOM	4391	OH0	WAT	X	50	26.960	36.851	6.038	1.00	44.57	8
ATOM	4392	OH1	WAT	X	50	37.082	59.754	36.774	1.00	66.16	8
ATOM	4393	OH2	WAT	X	50	57.220	36.380	35.486	1.00	60.08	8
ATOM	4394	OH3	WAT	X	50	47.460	48.140	35.950	1.00	51.89	8
ATOM	4395	OH4	WAT	X	50	32.642	7.671	29.024	1.00	62.58	8
ATOM	4396	OH5	WAT	X	50	40.898	5.278	12.690	1.00	58.65	8
ATOM	4397	OH6	WAT	X	50	43.951	11.795	23.808	1.00	51.02	8
ATOM	4398	OH7	WAT	X	50	56.331	38.665	59.400	1.00	77.23	8
ATOM	4399	OH8	WAT	X	50	42.112	15.859	19.271	1.00	42.44	8
ATOM	4400	OH9	WAT	X	51	43.751	9.508	10.207	1.00	72.09	8
ATOM	4401	OH1	WAT	X	51	21.156	18.175	-5.366	1.00	59.15	8
ATOM	4402	OH2	WAT	X	51	20.822	20.591	30.625	1.00	53.15	8
ATOM	4403	OH3	WAT	X	51	25.847	41.728	50.223	1.00	53.16	8
ATOM	4404	OH4	WAT	X	51	42.406	49.560	54.444	1.00	49.42	8
ATOM	4405	OH5	WAT	X	51	11.152	-0.096	4.529	1.00	73.12	8
ATOM	4406	OH6	WAT	X	51	41.064	10.519	39.198	1.00	76.33	8
ATOM	4407	OH7	WAT	X	51	11.838	45.652	24.174	1.00	52.20	8
ATOM	4408	OH8	WAT	X	51	24.803	8.502	38.134	1.00	48.46	8
ATOM	4409	OH9	WAT	X	51	28.241	55.029	32.933	1.00	56.81	8
ATOM	4410	OH0	WAT	X	52	24.326	46.042	48.362	1.00	42.89	8
ATOM	4411	OH1	WAT	X	52	60.372	23.243	57.581	1.00	51.46	8
ATOM	4412	OH2	WAT	X	52	44.063	13.149	3.195	1.00	73.23	8
ATOM	4413	OH3	WAT	X	52	29.959	38.273	7.993	1.00	74.96	8
ATOM	4414	OH4	WAT	X	52	17.959	47.341	32.823	1.00	52.58	8
ATOM	4415	OH5	WAT	X	52	35.761	36.887	7.808	1.00	46.76	8
ATOM	4416	OH6	WAT	X	52	29.185	14.140	50.554	1.00	100.00	8
ATOM	4417	OH7	WAT	X	52	46.852	47.409	54.235	1.00	47.47	8
ATOM	4418	OH8	WAT	X	52	46.124	18.871	10.000	1.00	74.45	8
ATOM	4419	OH9	WAT	X	52	43.467	42.127	14.225	1.00	58.70	8
ATOM	4420	OH0	WAT	X	53	42.354	10.824	26.570	1.00	74.16	8
ATOM	4421	OH1	WAT	X	53	41.382	9.160	28.416	1.00	65.06	8
ATOM	4422	OH2	WAT	X	53	32.249	16.276	51.085	1.00	66.53	8
ATOM	4423	OH3	WAT	X	53	43.754	20.935	55.297	1.00	89.21	8
ATOM	4424	OH4	WAT	X	53	46.525	22.435	61.833	1.00	64.40	8
ATOM	4425	OH5	WAT	X	53	36.689	9.501	46.403	1.00	43.78	8
ATOM	4426	OH6	WAT	X	53	13.785	14.234	21.394	1.00	46.49	8
ATOM	4427	OH7	WAT	X	53	44.108	8.308	6.121	1.00	74.38	8
ATOM	4428	OH8	WAT	X	53	37.095	13.297	47.553	1.00	92.89	8
ATOM	4429	OH9	WAT	X	54	60.222	38.361	56.675	1.00	71.18	8
ATOM	4430	OH0	WAT	X	54	43.676	52.104	52.067	1.00	52.01	8
ATOM	4431	OH1	WAT	X	54	13.472	23.519	26.526	1.00	85.06	8
ATOM	4432	OH2	WAT	X	54	26.573	48.774	55.241	1.00	63.24	8
ATOM	4433	OH3	WAT	X	54	38.373	54.655	25.877	1.00	61.51	8
ATOM	4434	OH4	WAT	X	54	40.109	29.004	7.323	1.00	50.80	8
ATOM	4435	OH5	WAT	X	54	40.897	28.228	33.474	1.00	55.10	8
ATOM	4436	OH6	WAT	X	54	26.359	57.407	32.671	1.00	74.31	8
ATOM	4437	OH7	WAT	X	54	15.383	36.694	13.336	1.00	63.49	8
ATOM	4438	OH8	WAT	X	55	25.637	23.526	51.791	1.00	62.36	8
ATOM	4439	OH9	WAT	X	55	47.868	37.197	21.724	1.00	98.01	8
ATOM	4440	OH0	WAT	X	55	48.664	28.592	20.875	1.00	61.42	8
ATOM	4441	OH1	WAT	X	55	22.182	11.543	42.550	1.00	50.93	8
ATOM	4442	OH2	WAT	X	55	14.290	33.767	23.519	1.00	43.45	8
ATOM	4443	OH3	WAT	X	55	49.254	21.261	57.388	1.00	74.77	8
ATOM	4444	OH4	WAT	X	55	32.072	50.437	56.442	1.00	84.60	8
ATOM	4445	OH5	WAT	X	55	6.861	26.478	7.012	1.00	69.24	8
ATOM	4446	OH6	WAT	X	55	36.069	6.771	2.277	1.00	89.64	8
ATOM	4447	OH7	WAT	X	55	60.239	29.387	37.677	1.00	64.46	8
ATOM	4448	OH8	WAT	X	56	46.693	15.300	46.504	1.00	37.40	8
ATOM	4449	OH9	WAT	X	56	47.685	47.802	26.981	1.00	44.40	8
ATOM	4450	OH0	WAT	X	56	21.472	47.007	15.910	1.00	70.01	8
ATOM	4451	OH1	WAT	X	56	2.967	21.682	5.603	1.00	60.74	8
ATOM	4452	OH2	WAT	X	56	62.723	25.567	58.195	1.00	45.51	8

4453	ATOH	OW6	WAT	X	56	53.874	20.460	35.843	1.00	60.27	8
4454	ATOH	OW7	WAT	X	56	34.063	6.968	31.691	1.00	54.01	8
4455	ATOH	OW8	WAT	X	56	20.830	41.835	12.224	1.00	100.00	8
4456	ATOH	OW9	WAT	X	56	16.599	30.946	13.916	1.00	37.38	8
4457	ATOH	OW0	WAT	X	57	44.358	21.696	24.084	1.00	64.44	8
4458	ATOH	OW1	WAT	X	57	9.788	43.318	30.716	1.00	90.76	8
4459	ATOH	OW2	WAT	X	57	65.207	28.476	57.189	1.00	72.19	8
4460	ATOH	OW3	WAT	X	57	20.871	4.547	-1.268	1.00	64.52	8
4461	ATOH	OW4	WAT	X	57	24.856	36.282	6.866	1.00	55.25	8
4462	ATOH	OW5	WAT	X	57	65.931	24.875	58.247	1.00	42.06	8
4463	ATOH	OW6	WAT	X	57	41.604	10.565	45.137	1.00	80.93	8
4464	ATOH	OW7	WAT	X	57	30.736	44.603	54.453	1.00	58.39	8
4465	ATOH	OW8	WAT	X	58	22.167	48.706	40.870	1.00	52.19	8
4466	ATOH	OW9	WAT	X	58	66.082	25.557	51.546	1.00	48.90	8
4467	ATOH	OW0	WAT	X	58	25.692	34.825	52.948	1.00	50.59	8
4468	ATOH	OW1	WAT	X	58	26.160	51.696	48.736	1.00	44.75	8
4469	ATOH	OW2	WAT	X	58	56.334	43.153	40.380	1.00	53.34	8
4470	ATOH	OW3	WAT	X	58	30.990	17.627	55.917	1.00	84.28	8
4471	ATOH	OW4	WAT	X	58	45.287	39.941	7.939	1.00	57.03	8
4472	ATOH	OW5	WAT	X	58	3.405	18.650	9.230	1.00	73.95	8
4473	ATOH	OW6	WAT	X	58	54.294	19.752	55.578	1.00	50.99	8
4474	ATOH	OW7	WAT	X	58	44.732	52.287	54.381	1.00	75.96	8
4475	ATOH	OW8	WAT	X	59	47.776	51.035	36.798	1.00	53.81	8
4476	ATOH	OW9	WAT	X	59	29.391	47.450	56.869	1.00	86.62	8
4477	ATOH	OW0	WAT	X	59	38.808	50.946	52.782	1.00	47.24	8
4478	ATOH	OW1	WAT	X	59	20.090	10.595	-7.477	1.00	69.34	8
4479	ATOH	OW2	WAT	X	59	30.700	10.315	45.674	1.00	63.75	8
4480	ATOH	OW3	WAT	X	59	60.018	46.795	44.900	1.00	57.35	8
4481	ATOH	OW4	WAT	X	59	46.214	52.834	49.312	1.00	67.99	8
4482	ATOH	OW5	WAT	X	59	56.880	28.891	60.457	1.00	85.53	8
4483	ATOH	OW6	WAT	X	59	36.280	48.379	58.178	1.00	71.18	8
4484	ATOH	OW7	WAT	X	59	35.313	2.318	16.129	1.00	66.51	8
4485	ATOH	OW8	WAT	X	60	34.944	58.828	34.422	1.00	69.27	8
4486	ATOH	OW9	WAT	X	60	47.891	40.270	60.882	1.00	62.61	8
4487	ATOH	OW0	WAT	X	60	20.100	54.046	30.414	1.00	91.37	8
4488	ATOH	OW1	WAT	X	60	0.668	22.084	15.126	1.00	45.99	8
4489	ATOH	OW2	WAT	X	60	50.911	50.933	54.227	1.00	71.78	8
4490	ATOH	OW3	WAT	X	60	50.514	44.428	38.574	1.00	67.41	8
4491	ATOH	OW4	WAT	X	60	31.208	54.171	26.648	1.00	65.99	8
4492	ATOH	OW5	WAT	X	60	49.541	38.319	60.498	1.00	49.78	8
4493	ATOH	OW6	WAT	X	60	23.270	55.339	31.653	1.00	66.17	8
4494	ATOH	OW7	WAT	X	60	46.551	15.109	50.163	1.00	87.28	8
4495	ATOH	OW8	WAT	X	61	65.999	24.860	47.686	1.00	57.42	8
4496	ATOH	OW9	WAT	X	61	30.573	36.197	57.967	1.00	51.73	8
4497	ATOH	OW0	WAT	X	61	3.779	13.380	-2.503	1.00	65.73	8
4498	ATOH	OW1	WAT	X	61	48.944	12.221	41.061	1.00	39.29	8
4499	ATOH	OW2	WAT	X	61	64.745	25.656	43.289	1.00	52.05	8
4500	ATOH	OW3	WAT	X	61	51.657	40.026	13.448	1.00	68.71	8
4501	ATOH	OW4	WAT	X	61	27.718	47.942	52.615	1.00	54.81	8
4502	ATOH	OW5	WAT	X	61	24.460	41.243	12.842	1.00	65.85	8
4503	ATOH	OW6	WAT	X	61	2.848	14.406	12.411	1.00	61.94	8
4504	ATOH	OW7	WAT	X	62	23.747	48.989	47.991	1.00	55.02	8
4505	ATOH	OW8	WAT	X	62	63.167	23.291	45.841	1.00	64.42	8
4506	ATOH	OW9	WAT	X	62	55.731	29.439	38.673	1.00	64.37	8
4507	ATOH	OW0	WAT	X	62	39.039	4.879	14.767	1.00	52.29	8
4508	ATOH	OW1	WAT	X	62	43.782	27.030	47.614	1.00	5.00	8
4509	ATOH	OW2	WAT	X	62	27.765	34.219	1.860	1.00	67.67	8
4510	ATOH	OW3	WAT	X	62	65.774	20.800	46.451	1.00	72.56	8
4511	ATOH	OW4	WAT	X	63	65.823	27.727	48.583	1.00	52.36	8
4512	ATOH	OW5	WAT	X	63	47.510	11.024	43.713	1.00	70.64	8
4513	ATOH	OW6	WAT	X	63	66.150	30.203	50.411	1.00	51.22	8
4514	ATOH	OW7	WAT	X	63	48.889	20.346	31.711	1.00	85.43	8
4515	ATOH	OW8	WAT	X	63	16.744	26.725	47.695	1.00	75.57	8
4516	ATOH	OW9	WAT	X	63	19.203	31.730	8.203	1.00	81.36	8
4517	ATOH	OW0	WAT	X	63	18.178	51.891	26.673	1.00	67.60	8
4518	ATOH	OW1	WAT	X	63	31.035	55.837	30.147	1.00	68.28	8
4519	ATOH	OW2	WAT	X	64	34.256	54.728	25.341	1.00	80.95	8
4520	ATOH	OW3	WAT	X	64	44.621	47.771	25.528	1.00	59.54	8
4521	ATOH	OW4	WAT	X	64	16.999	27.936	51.121	1.00	61.68	8
4522	ATOH	OW5	WAT	X	64	36.358	38.943	11.274	1.00	52.06	8
4523	ATOH	OW6	WAT	X	64	16.404	22.381	39.229	1.00	36.64	8
4524	ATOH	OW7	WAT	X	64	23.799	46.745	46.122	1.00	69.59	8
4525	ATOH	OW8	WAT	X	64	30.457	7.355	-1.129	1.00	72.94	8
4526	ATOH	OW9	WAT	X	65	19.222	33.502	3.190	1.00	50.09	8
4527	ATOH	OW0	WAT	X	65	46.509	18.371	25.238	1.00	62.10	8
4528	ATOH	OW1	WAT	X	65	32.283	10.295	-4.119	1.00	66.36	8
4529	ATOH	OW2	WAT	X	65	11.959	41.211	33.089	1.00	76.54	8
4530	ATOH	OW3	WAT	X	65	19.983	24.472	46.573	1.00	65.57	8
4531	ATOH	OW4	WAT	X	65	9.603	26.690	3.912	1.00	75.52	8
4532	ATOH	OW5	WAT	X	66	45.825	9.757	40.836	1.00	72.28	8
4533	ATOH	OW6	WAT	X	66	49.404	34.287	20.920	1.00	61.42	8
4534	ATOH	OW7	WAT	X	66	21.346	51.355	35.980	1.00	76.73	8
4535	ATOH	OW8	WAT	X	66	34.793	9.610	-4.714	1.00	67.39	8
4536	ATOH	OW9	WAT	X	66	6.006	27.070	13.534	1.00	83.61	8
4537	ATOH	OW0	WAT	X	67	57.091	33.822	60.700	1.00	78.52	8
4538	ATOH	OW1	WAT	X	67	3.688	25.711	4.813	1.00	69.62	8
4539	ATOH	OW2	WAT	X	67	11.853	27.880	7.921	1.00	58.69	8
4540	ATOH	OW3	WAT	X	67	35.486	56.715	40.693	1.00	63.30	8
4541	ATOH	OW4	WAT	X	67	20.467	20.497	41.249	1.00	43.89	8
4542	ATOH	OW5	WAT	X	67	37.508	57.667	34.228	1.00	69.67	8
4543	ATOH	OW6	WAT	X	68	8.621	27.294	14.147	1.00	55.12	8
4544	ATOH	OW7	WAT	X	68	3.733	19.033	3.659	1.00	55.87	8
4545	ATOH	OW8	WAT	X	68	18.954	18.854	32.541	1.00	67.33	8
4546	ATOH	OW9	WAT	X	68	25.346	2.504	4.877	1.00	66.26	8
4547	ATOH	OW0	WAT	X	68	34.927	1.355	1.837	1.00	61.60	8
4548	ATOH	OW1	WAT	X	68	47.719	47.565	30.106	1.00	67.71	8
4549	ATOH	OW2	WAT	X	68	58.933	17.613	53.979	1.00	65.35	8
4550	ATOH	OW3	WAT	X	69	16.418	40.606	47.124	1.00	61.68	8
4551	ATOH	OW4	WAT	X	69	33.051	35.235	6.368	1.00	63.11	8
4552	ATOH	OW5	WAT	X	69	10.404	2.233	-1.826	1.00	71.56	8
4553	ATOH	OW6	WAT	X	69	27.844	10.427	43.773	1.00	65.38	8
4554	ATOH	OW7	WAT	X	69	9.821	19.794	23.580	1.00	74.16	8
4555	ATOH	OW8	WAT	X	69	34.906	24.545	27.529	1.00	77.66	8
4556	ATOH	OW9	WAT	X	69	42.873	50.265	43.593	1.00	82.51	8
4557	ATOH	OW0	WAT	X	70	11.780	40.835	20.822	1.00	57.23	8
4558	ATOH	OW1	WAT	X	70	23.833	50.272	22.080	1.00	57.23	8

ATOH	4559	0W3	WAT	X	70	12.149	0.500	-0.175	1.00100.00	8	ATOH	4612	0W2	WAT	X	81	13.341	34.872	38.349	1.00	64.64	8	
ATOH	4560	0W4	WAT	X	70	24.781	48.147	16.489	1.00	53.74	8	ATOH	4613	0W3	WAT	X	81	51.626	42.754	59.455	1.00	87.45	8
ATOH	4561	0W5	WAT	X	70	45.295	18.629	15.166	1.00	66.52	8	ATOH	4614	0W5	WAT	X	81	17.748	40.786	43.576	1.00	81.62	8
ATOH	4562	0W8	WAT	X	70	16.273	24.172	43.929	1.00	86.28	8	ATOH	4615	0W6	WAT	X	81	40.981	31.297	32.687	1.00	92.90	8
ATOH	4563	0W2	WAT	X	71	14.692	0.299	4.588	1.00	76.24	8	ATOH	4616	0W7	WAT	X	81	36.339	42.304	57.906	1.00	54.44	8
ATOH	4564	0W3	WAT	X	71	56.655	45.988	46.443	1.00	74.53	8	ATOH	4617	0W0	WAT	X	82	52.150	44.557	55.907	1.00	81.29	8
ATOH	4565	0W4	WAT	X	71	44.653	15.572	21.500	1.00	81.92	8	ATOH	4618	0W1	WAT	X	82	44.696	27.699	29.800	1.00	66.84	8
ATOH	4566	0W6	WAT	X	71	13.915	34.012	32.549	1.00	76.95	8	ATOH	4619	0W2	WAT	X	82	15.369	42.073	36.641	1.00	87.69	8
ATOH	4567	0W1	WAT	X	72	18.894	23.324	28.037	1.00	69.01	8	ATOH	4620	0W4	WAT	X	82	44.262	38.613	61.725	1.00	74.79	8
ATOH	4568	0W2	WAT	X	72	25.942	27.526	52.380	1.00	57.92	8	ATOH	4621	0W5	WAT	X	82	10.887	37.555	22.160	1.00	77.71	8
ATOH	4569	0W3	WAT	X	72	20.444	43.760	44.743	1.00	57.92	8	ATOH	4622	0W6	WAT	X	82	57.317	26.895	38.482	1.00	54.04	8
ATOH	4570	0W5	WAT	X	72	56.463	15.927	56.362	1.00	90.66	8	ATOH	4623	0W1	WAT	X	83	1.485	10.546	14.639	1.00	49.60	8
ATOH	4571	0W6	WAT	X	72	67.258	38.530	40.380	1.00	71.85	8	ATOH	4624	0W2	WAT	X	83	44.383	11.585	44.954	1.00	69.75	8
ATOH	4572	0W2	WAT	X	73	13.119	23.916	-2.569	1.00	67.91	8	ATOH	4625	0W4	WAT	X	83	13.091	19.080	23.540	1.00	84.10	8
ATOH	4573	0W3	WAT	X	73	27.753	4.319	2.523	1.00	68.14	8	ATOH	4626	0W5	WAT	X	83	49.664	18.609	50.424	1.00	79.36	8
ATOH	4574	0W4	WAT	X	73	15.049	27.612	26.046	1.00	71.85	8	ATOH	4627	0W6	WAT	X	83	-0.411	-0.186	6.219	1.00	73.91	8
ATOH	4575	0W7	WAT	X	73	41.506	30.331	28.071	1.00	39.96	8	ATOH	4628	0W1	WAT	X	84	-0.060	12.467	10.762	1.00	74.36	8
ATOH	4576	0W9	WAT	X	73	49.356	13.175	50.180	1.00	77.21	8	ATOH	4629	0W3	WAT	X	84	45.916	18.172	53.625	1.00	82.88	8
ATOH	4577	0W0	WAT	X	74	44.776	9.064	36.247	1.00	56.22	8	ATOH	4630	0W4	WAT	X	84	42.886	23.516	61.123	1.00	71.70	8
ATOH	4578	0W2	WAT	X	74	14.995	33.147	12.393	1.00	74.77	8	ATOH	4631	0W5	WAT	X	84	26.711	5.741	19.232	1.00	65.61	8
ATOH	4579	0W3	WAT	X	74	21.394	18.527	43.796	1.00	77.10	8	ATOH	4632	0W6	WAT	X	84	18.341	21.188	47.071	1.00	79.82	8
ATOH	4580	0W4	WAT	X	74	0.275	3.244	2.071	1.00	89.93	8	ATOH	4633	0W8	WAT	X	84	30.324	37.244	55.283	1.00	63.21	8
ATOH	4581	0W5	WAT	X	74	32.705	3.566	1.290	1.00	100.00	8	ATOH	4634	0W9	WAT	X	84	45.383	21.545	29.439	1.00	65.08	8
ATOH	4582	0W6	WAT	X	74	23.871	44.907	16.023	1.00	71.10	8	ATOH	4635	0W1	WAT	X	85	47.617	21.423	28.329	1.00	72.90	8
ATOH	4583	0W8	WAT	X	74	41.289	9.005	3.932	1.00	71.97	8	ATOH	4636	0W2	WAT	X	85	14.724	8.133	-4.054	1.00	80.41	8
ATOH	4584	0W2	WAT	X	75	38.329	57.673	44.241	1.00	64.90	8	ATOH	4637	0W4	WAT	X	85	14.404	38.900	34.440	1.00	73.60	8
ATOH	4585	0W5	WAT	X	75	18.910	30.958	52.593	1.00	93.30	8	ATOH	4638	0W5	WAT	X	85	30.311	39.411	56.032	1.00	72.07	8
ATOH	4586	0W6	WAT	X	75	68.020	36.610	50.288	1.00	86.49	8	ATOH	4639	0W1	WAT	X	86	38.750	51.931	56.443	1.00	83.88	8
ATOH	4587	0W2	WAT	X	76	22.139	39.199	7.275	1.00	71.53	8	ATOH	4640	0W2	WAT	X	86	28.737	50.755	56.620	1.00	78.91	8
ATOH	4588	0W3	WAT	X	76	58.720	42.672	38.660	1.00	68.73	8	ATOH	4641	0W3	WAT	X	86	38.447	9.203	1.111	1.00	60.02	8
ATOH	4589	0W5	WAT	X	76	61.482	44.540	47.192	1.00	77.48	8	ATOH	4642	0W4	WAT	X	86	63.955	18.750	55.290	1.00	75.30	8
ATOH	4590	0W9	WAT	X	76	22.107	41.072	47.776	1.00	60.73	8	ATOH	4643	0W5	WAT	X	86	28.437	41.435	56.329	1.00	77.99	8
ATOH	4591	0W2	WAT	X	77	2.634	-1.318	3.949	1.00	69.96	8	ATOH	4644	0W6	WAT	X	86	27.951	49.707	19.814	1.00	80.66	8
ATOH	4592	0W3	WAT	X	77	32.187	5.643	25.223	1.00	76.13	8	ATOH	4645	0W7	WAT	X	86	33.978	8.299	40.249	1.00	69.22	8
ATOH	4593	0W4	WAT	X	77	67.602	33.066	51.363	1.00	72.25	8	ATOH	4646	0W9	WAT	X	86	17.498	1.498	10.616	1.00	71.37	8
ATOH	4594	0W5	WAT	X	77	52.748	50.627	48.547	1.00	74.39	8	ATOH	4647	0W1	WAT	X	87	1.278	15.798	6.438	1.00	70.87	8
ATOH	4595	0W6	WAT	X	77	10.204	44.509	25.769	1.00	64.94	8	ATOH	4648	0W3	WAT	X	87	37.174	55.549	52.513	1.00	69.91	8
ATOH	4596	0W7	WAT	X	77	22.754	10.234	24.846	1.00	66.60	8	ATOH	4649	0W4	WAT	X	87	68.146	21.047	55.397	1.00	70.79	8
ATOH	4597	0W2	WAT	X	78	65.372	34.387	54.026	1.00	68.26	8	ATOH	4650	0W5	WAT	X	87	24.655	52.548	24.459	1.00	72.31	8
ATOH	4598	0W3	WAT	X	78	61.952	23.010	40.260	1.00	64.44	8	ATOH	4651	0W6	WAT	X	87	46.009	24.086	33.287	1.00	79.02	8
ATOH	4599	0W4	WAT	X	78	6.141	-0.725	6.920	1.00	63.43	8	ATOH	4652	0W9	WAT	X	87	50.195	14.529	36.835	1.00	65.15	8
ATOH	4600	0W6	WAT	X	78	62.946	40.127	37.159	1.00	64.61	8	ATOH	4653	0W2	WAT	X	88	29.201	3.240	-2.272	1.00	78.74	8
ATOH	4601	0W2	WAT	X	79	57.524	45.787	43.333	1.00	68.47	8	ATOH	4654	0W3	WAT	X	88	13.357	32.036	24.857	1.00	62.05	8
ATOH	4602	0W3	WAT	X	79	27.601	6.844	22.540	1.00	100.00	8	ATOH	4655	0W4	WAT	X	88	65.406	20.886	50.995	1.00	73.98	8
ATOH	4603	0W4	WAT	X	79	13.772	31.115	20.743	1.00	57.33	8	ATOH	4656	0W5	WAT	X	88	20.515	8.228	19.759	1.00	76.49	8
ATOH	4604	0W5	WAT	X	79	58.663	23.880	36.310	1.00	71.62	8	ATOH	4657	0W6	WAT	X	88	46.758	18.587	30.455	1.00	74.75	8
ATOH	4605	0W6	WAT	X	79	49.511	45.784	34.237	1.00	64.41	8	ATOH	4658	0W2	WAT	X	89	49.679	43.124	20.824	1.00	80.84	8
ATOH	4606	0W3	WAT	X	80	42.349	10.479	16.376	1.00	86.89	8	ATOH	4659	0W3	WAT	X	89	60.303	44.435	40.737	1.00	70.62	8
ATOH	4607	0W2	WAT	X	80	64.430	36.390	57.479	1.00	81.60	8	ATOH	4660	0W4	WAT	X	89	13.240	-1.159	9.184	1.00	78.53	8
ATOH	4608	0W4	WAT	X	80	51.348	32.222	6.850	1.00	86.83	8	ATOH	4661	0W5	WAT	X	89	61.700	19.538	53.061	1.00	64.93	8
ATOH	4609	0W6	WAT	X	80	28.165	8.846	38.088	1.00	71.08	8	ATOH	4662	0W6	WAT	X	89	24.291	28.301	0.472	1.00	69.68	8
ATOH	4610	0W8	WAT	X	80	65.757	27.493	53.760	1.00	48.10	8	ATOH	4663	0W0	WAT	X	90	27.964	24.098	-2.600	1.00	64.61	8
ATOH	4611	0W1	WAT	X	81	45.249	12.674	37.874	1.00	50.64	8	ATOH	4664	0W1	WAT	X	90	22.140	24.413	52.912	1.00	67.47	8

ATOH	4665	OW3	WAT	X	90	39.112	6.740	5.054	1.00	66.72	8
ATOH	4666	OW4	WAT	X	90	43.364	57.890	49.964	1.00	71.30	8
ATOH	4667	OW6	WAT	X	90	16.187	17.842	27.844	1.00	71.63	8
ATOH	4668	OW7	WAT	X	90	22.913	3.223	6.101	1.00	63.34	8
ATOH	4669	OW0	WAT	X	91	0.373	23.417	18.644	1.00	68.95	8
ATOH	4670	OW1	WAT	X	91	19.144	22.297	52.147	1.00	68.45	8
ATOH	4671	OW2	WAT	X	91	46.750	22.374	17.228	1.00	68.56	8
ATOH	4672	OW3	WAT	X	91	50.310	39.246	9.155	1.00	68.48	8
ATOH	4673	OW5	WAT	X	91	14.832	31.811	-1.674	1.00	65.32	8
ATOH	4674	OW6	WAT	X	91	39.568	22.971	59.682	1.00	94.75	8
ATOH	4675	OW0	WAT	X	92	28.305	37.474	53.688	1.00	64.82	8
ATOH	4676	OW1	WAT	X	92	60.842	35.037	35.557	1.00	68.20	8
ATOH	4677	OW3	WAT	X	92	38.306	2.043	9.940	1.00	74.71	8
ATOH	4678	OW4	WAT	X	92	37.932	10.010	23.873	1.00	62.54	8
ATOH	4679	OW5	WAT	X	92	37.872	59.284	31.560	1.00	64.40	8
ATOH	4680	OW8	WAT	X	92	16.587	37.900	45.458	1.00	57.48	8
ATOH	4681	OW2	WAT	X	93	24.426	6.991	31.450	1.00	62.04	8
ATOH	4682	OW3	WAT	X	93	15.322	46.823	24.885	1.00	68.48	8
ATOH	4683	OW5	WAT	X	93	18.754	23.194	42.946	1.00	69.72	8
ATOH	4684	OW6	WAT	X	93	20.937	46.805	43.439	1.00	65.25	8
ATOH	4685	OW8	WAT	X	93	28.767	42.761	53.085	1.00	51.35	8
ATOH	4686	OW0	WAT	X	94	32.517	16.473	33.381	1.00	60.16	8
ATOH	4687	OW2	WAT	X	94	26.635	4.800	29.351	1.00	63.33	8
ATOH	4688	OW3	WAT	X	94	1.194	4.216	9.172	1.00	60.36	8
ATOH	4689	OW4	WAT	X	94	25.652	19.885	-5.299	1.00	58.09	8
ATOH	4690	OW5	WAT	X	94	43.661	12.692	20.184	1.00	65.23	8
ATOH	4691	OW6	WAT	X	94	17.439	46.586	41.518	1.00	66.21	8
ATOH	4692	OW7	WAT	X	94	35.133	15.487	30.639	1.00	49.75	8
ATOH	4693	OW8	WAT	X	94	36.346	8.698	18.844	1.00	48.58	8
ATOH	4694	OW0	WAT	X	95	30.818	8.165	40.656	1.00	56.86	8
ATOH	4695	OW1	WAT	X	95	40.089	21.776	55.765	1.00	53.69	8
ATOH	4696	OW2	WAT	X	95	18.639	14.065	-5.612	1.00	55.94	8
ATOH	4697	OW3	WAT	X	95	51.587	38.457	41.331	1.00	56.04	8
ATOH	4698	OW4	WAT	X	95	50.107	29.401	17.255	1.00	56.00	8
ATOH	4699	OW5	WAT	X	95	8.218	14.744	20.596	1.00	56.95	8
ATOH	4700	OW6	WAT	X	95	40.674	47.760	57.927	1.00	54.91	8

CLAIMS

1. A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and at least
5 one altered property as compared to said parent α -amylase, which method comprises

i) analysing the structure of the parent Termamyl-like α -amylase to identify at least one amino acid residue or at least
10 one structural part of the Termamyl-like α -amylase structure, which amino acid residue or structural part is believed to be of relevance for altering said property of the parent Termamyl-like α -amylase (as evaluated on the basis of structural or functional considerations),

15

ii) constructing a Termamyl-like α -amylase variant, which as compared to the parent Termamyl-like α -amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

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iii) testing the resulting Termamyl-like α -amylase variant for said property.

2. The method according to claim 1, wherein the property to be
25 altered is selected from the group consisting of substrate specificity, substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6) or high (e.g. pH>9) pH values), stability towards oxidation, Ca^{2+} -
30 dependency and specific activity.

3. The method according to claim 1 or 2, wherein the property to be altered is the calcium ion dependency and the structural part to be modified is selected from the group consisting of
35 the C domain, the interface between the A and B domain, the interface between the A and C domain, or the interaction to a calcium binding site of the Termamyl-like α -amylase.

4. The method according to claim 1 or 2, wherein the property to be altered is the substrate cleavage pattern and the structural part to be modified is located within 10Å from an amino acid residue of the substrate binding site.

5

5. A method of constructing a variant of a parent Termamyl-like α -amylase, which variant has α -amylase activity and one or more altered properties as compared to said parent α -amylase, which method comprises

10 i) comparing the three-dimensional structure of the Termamyl-like α -amylase with the structure of a non-Termamyl-like α -amylase,

ii) identifying a part of the Termamyl-like α -amylase structure which is different from the non-Termamyl-like α -amylase
15 structure and which from structural or functional considerations is contemplated to be responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α -amylase, and

iii) modifying the part of the Termamyl-like α -amylase
20 identified in ii) whereby a Termamyl-like α -amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α -amylase.

6. The method according to claim 6, wherein, in step iii), the
25 part of the Termamyl-like α -amylase is modified so as to resemble the corresponding part of the non-Termamyl-like α -amylase.

7. The method according to claim 5 or 6, wherein, in step iii),
30 the modification is accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified; by replacing one or more amino acid residues of the part of the Termamyl-like α -amylase to be modified with the amino acid residues occupying corresponding positions in the
35 non-Termamyl-like α -amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α -amylase into a corresponding position in the Termamyl-like α -amylase.

8. The method according to any of claims 5-7, wherein the non-Termamyl-like α -amylase structure is the structure of a fungal α -amylase or a mammalian α -amylase.
- 5 9. The method according to claim 8, wherein the non-Termamyl-like α -amylase is the *Aspergillus oryzae* TAKA α -amylase, the *A. niger* acid α -amylase, the *Bacillus subtilis* α -amylase or the pig pancreatic α -amylase.
- 10 10. The method according to any of claims 1-9, wherein the parent Termamyl-like α -amylase is derived from a strain of *Bacillus*.
11. The method according to claim 10, wherein the parent α -
15 amylase is derived from a strain of a *B. licheniformis*, *B. amyloliquefaciens*, *B. stearothermophilus* or a strain from an alkalophilic *Bacillus* sp. such as NCIB 12289, NCIB 12512 or NCIB 12513.
- 20 12. The method according to any of claims 1-11, wherein the parent α -amylase is a hybrid α -amylase comprising a combination of partial amino acid sequences derived from at least two α -amylases, of which one is a Termamyl-like α -amylase and the other(s) are, e.g., from a microbial and/or a mammalian α -
25 amylase.
13. The method according to any of claims 5-12, wherein the part of the parent Termamyl-like α -amylase to be modified and identified in step ii) is loop 1, loop 2, loop 3 and/or loop 8
30 of the parent α -amylase.
13. A method of constructing a variant of a parent Termamyl-like α -amylase, which has a decreased calcium ion dependency as compared to said parent, which method comprises:
35
- i) identifying an amino acid residue within 10Å from a Ca^{2+} binding site of a Termamyl-like α -amylase in a model of the three-dimensional structure of said α -amylase, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,

- ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and
- iii) testing the Ca^{2+} dependency of the resulting Termamyl-like α -amylase variant.

10 14. A method of constructing a variant of a parent Termamyl-like α -amylase which variant has α -amylase activity and an altered pH dependent activity, which method comprises

- i) in a three-dimensional structure of the Termamyl-like α -amylase in question, identifying an amino acid residue within 15Å from an active site residue, in particular 10Å from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue,

- 20 ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and evaluating the accomodation of the amino acid residue in the structure,

- iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into the structure,

- 30 iv) constructing a Termamyl-like α -amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent activity of said variant.

35 15. A method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α -amylase, which method comprises

- i) identifying an internal hole or a crevice of the parent Termamyl-like α -amylase in the three-dimensional structure of said α -amylase,
- ii) replacing, in the structure, one or more amino acid residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of the hole or crevice,
- 10 iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.

16. A method of constructing a variant of a Termamyl-like α -
15 amylase which has a reduced ability to cleave a substrate close to the branching point, which method comprises

- i) identifying the substrate binding area of the parent Termamyl-like α -amylase in a model of the three-dimensional
20 structure of said α -amylase,
- ii) replacing, in the model, one or more amino acid residues of the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of
25 the parent α -amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding
30 one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and
- iii) constructing a Termamyl-like α -amylase variant resulting from step ii) and testing the substrate cleavage pattern of the
35 variant.

17. The method according to any of the preceeding claims, in which the α -amylase variant is obtained by cultivating a

microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth.

5

18. A variant of a parent Termamyl-like α -amylase, in which variant at least one amino acid residue of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ
10 ID No. 4, has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of
15 SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

19. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of
20 variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No
25 10, wherein

X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,

30 Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and

V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

35 20. The variant according to claim 18 or 19, wherein X is the amino acid residue occupying position 48 and Y the amino acid residue occupying position 51 of SEQ ID NO 4 and Z is the amino

acid residue occupying position 70 and V the amino acid residue occupying position 78 in SEQ ID No 10.

21. A variant of a parent Termamyl-like α -amylase, in which
5 variant at least one of the amino acid residues of the parent
 α -amylase, which is/are present in an amino acid fragment
corresponding to the amino acid fragment 195-202 of the amino
acid sequence of SEQ ID No. 4, has been deleted or replaced
10 with one or more of the amino acid residues which is/are
present in an amino acid fragment corresponding to the amino
acid fragment 165-177 of the amino acid sequence shown in SEQ
ID No. 10, or in which one or more additional amino acid
residues has been added using the relevant part of SEQ ID No.
10 or a corresponding part of another Fungamyl-like α -amylase
15 as a template.

22. A variant of a parent Termamyl-like α -amylase, which
variant has a region which, when the amino acid sequence of
variant is aligned most closely with the amino acid sequence of
20 the said parent α -amylase, occupies the same position as the
portion from residue X to residue Y of SEQ ID No 4, the said
region having at least 80%, such as 90% sequence homology with
the part of SEQ ID No 10 extending from residue Z to residue V
of SEQ ID No 10, wherein
25 X is the amino acid occupying position 195 or 196 of SEQ ID No.
4,

Y is the amino acid residue occupying position 198, 199, 200,
201, or 202 of SEQ ID No. 4,

30

Z is the amino acid residue occupying position 165 or 166 of
SEQ ID No. 10, and

V is the amino acid residue occupying position 173, 174, 175,
35 176 or 177 of SEQ ID No. 10.

23. The variant according to claim 21 or 22, in which the amino
acid fragment of the parent α -amylase, which corresponds to

amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

5

24. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of
10 SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added
15 using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

25. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of
20 variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue
25 Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

30 Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

35

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

26. The variant according to claim 24 or 25, in which an amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

27. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

20

28. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

29. The variant according to claim 27 or 28, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

10

30. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

31. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No. 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No. 10 extending from residue Z to residue V of SEQ ID No. 10, wherein

X is the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

Y is the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

35 Z is the amino acid occupying position 28, 29, 30, 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

32. The variant according to claim 30 or 31, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

33. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

34. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein X is the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,

Z is the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

35

V is the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

35. The variant according to claim 33 or 34, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

36. A variant of a parent Termamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent α -amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α -amylase as a template.

37. A variant of a parent Termamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 2, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

Y is the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

38. The variant according to claim 36 or 37, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid
s residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

39. A variant of a parent Fungamyl-like α -amylase, in which variant at least one of the amino acid residues of the parent
10 α -amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid
15 residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α -amylase as a template.

20

40. A variant of a parent Fungamyl-like α -amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α -amylase, occupies the same position as the
25 portion from residue X to residue Y of SEQ ID No 10, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 4, wherein

X is the amino acid occupying position 117, 118, 119, 120 or
30 121 of SEQ ID No. 10,

Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

35 Z is the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

41. The variant according to claim 39 or 40, in which the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

10

42. A variant according to any of claims 39-41, in which the the amino acid fragment of the parent α -amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 4.

43. A variant of a parent Fungamyl-like α -amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the amino acid sequence shown in SEQ ID No. 10 has been deleted.

45. A variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a decreased Ca^{2+} dependency as compared to the parent α -amylase.

46. A variant according to claim 45, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID NO 2:

30 N104, A349, I479, L346, I430, N457, K385, F350, I411, H408 or G303, in particular a mutation corresponding to

N104D;

A349C+I479C;

L346C+I430C;

35 N457D,E;

N457D,E+K385R;

F350D,E+I430R,K;

F350D,E+I411R,K;

H408Q,E,N,D; and/or
G303N,D,Q,E.

47. A variant of a parent Termamyl-like α -amylase which
5 exhibits a higher activity below the pH optimum than the parent
 α -amylase, which variant comprises a mutation of an amino acid
residue corresponding to at least one of the following
positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):
E336, Q333, P331, I236, V102, A232, I103, L196, in particular
10 at least one of the following mutations:

E336R,K;
Q333R,K; P331R,K;
V102R,K,A,T,S,G;
I236K,R,N;
15 I103K,R;
L196K,R; and/or
A232T,S,G.

48. A variant of a parent Termamyl-like α -amylase which
20 exhibits a higher activity above the pH optimum than the parent
 α -amylase, which variant comprises a mutation of an amino acid
residue corresponding to at least one of the following
positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):
N236, H281 and/or Y273, in particular one of the following
25 mutations:

N326I,Y,F,L,V;
H281F,I,L; and/or
Y273F,W.

30 49. A variant of a parent Termamyl-like α -amylase which
exhibits α -amylase activity and which has an increased
thermostability and/or altered temperature optimum as compared
to the parent α -amylase, which variant comprises a mutation of
an amino acid residue corresponding to at least one of the
35 following positions of the *B. licheniformis* α -amylase (SEQ ID
NO 2):

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143, R146, L241, I236, L7, V259, F284, F350, F343, L427 and/or V481, in particular at least one of the following mutations:

L61W,V,F;

5 Y62W;

F67W;

K106R,F,W;

G145F,W

I212F,L,W,Y,R,K;

10 S151 replaced with any other amino acid residue and in particular with F,W,I or L;

R214W;

Y150R,K;

F143W;

15 R146W;

L241I,F,Y,W;

I236L,F,W,Y;

L7F,I,W;

V259F,I,L;

20 F284W;

F350W;

F343W;

L427F,L,W; and/or

V481,F,I,L,W.

25

50. A variant of a parent Termamyl-like α -amylase, which exhibits α -amylase activity and which has a reduced capability of cleaving an oligo-saccharide substrate close to the branching point as compared to the parent α -amylase, which
30 variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α -amylase (SEQ ID NO 2):

V54, D53, Y56, Q333 and/or G57, in particular at least one of
35 the following mutations:

V54L,I,F,Y,W,R,K,H,E,Q;

D53L,I,F,Y,W;

Y,56W;

Q333W; and/or

G57 to all possible amino acid residues.

51. The variant according to any of claims 17-50, wherein one
5 or more proline residues present in the amino acid residues
with which the parent α -amylase is modified are replaced with
a non-proline residue such as alanine.

52. The variant according to any of claims 17-51, wherein one
10 or more cysteine residues present in the amino acid residues
with which the parent α -amylase is modified are replaced with
a non-cysteine residue such as alanine.

53. A DNA construct comprising a DNA sequence encoding an α -
15 amylase variant according to any of claims 17-52.

54. A recombinant expression vector which carries a DNA con-
struct according to Claim 53.

20 55. A cell which is transformed with a DNA construct according
to Claim 53 or a vector according to Claim 54.

56. A cell according to Claim 55, which is a microorganism.

25 57. A cell according to Claim 56, which is a bacterium or a
fungus.

58. The cell according to Claim 57, which is a grampositive
bacterium such as *Bacillus subtilis*, *Bacillus licheniformis*,
30 *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*,
Bacillus alkalophilus, *Bacillus amyloliquefaciens*, *Bacillus*
coagulans, *Bacillus circulans*, *Bacillus lautus* or *Bacillus thu-*
ringiensis.

35 59. Use of an α -amylase variant according to any of claims 17-
52 for washing and/or dishwashing.

60. Use of an α -amylase variant according to any of claims 17-52 for desizing.
61. Use of an α -amylase variant according to any of claims 17-52 for starch liquefaction.
62. A detergent additive comprising an α -amylase variant according to any of claims 17-52, optionally in the form of a non-dusting granulate, stabilised liquid or protected enzyme.
63. A detergent additive according to Claim 62 which contains 0.02-200 mg of enzyme protein/g of the additive.
64. A detergent additive according to Claim 62 or 63, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.
65. A detergent composition comprising an α -amylase variant according to any of claims 17-52.
66. A detergent composition according to Claim 65 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.
67. A manual or automatic dishwashing detergent composition comprising an α -amylase variant according to any of claims 17-52.
68. A dishwashing detergent composition according to Claim 67 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.
69. A manual or automatic laundry washing composition comprising an α -amylase variant according to any of claims 17-52.

70. A laundry washing composition according to Claim 69, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, an amylolytic enzyme and/or a cellulase.

1/11

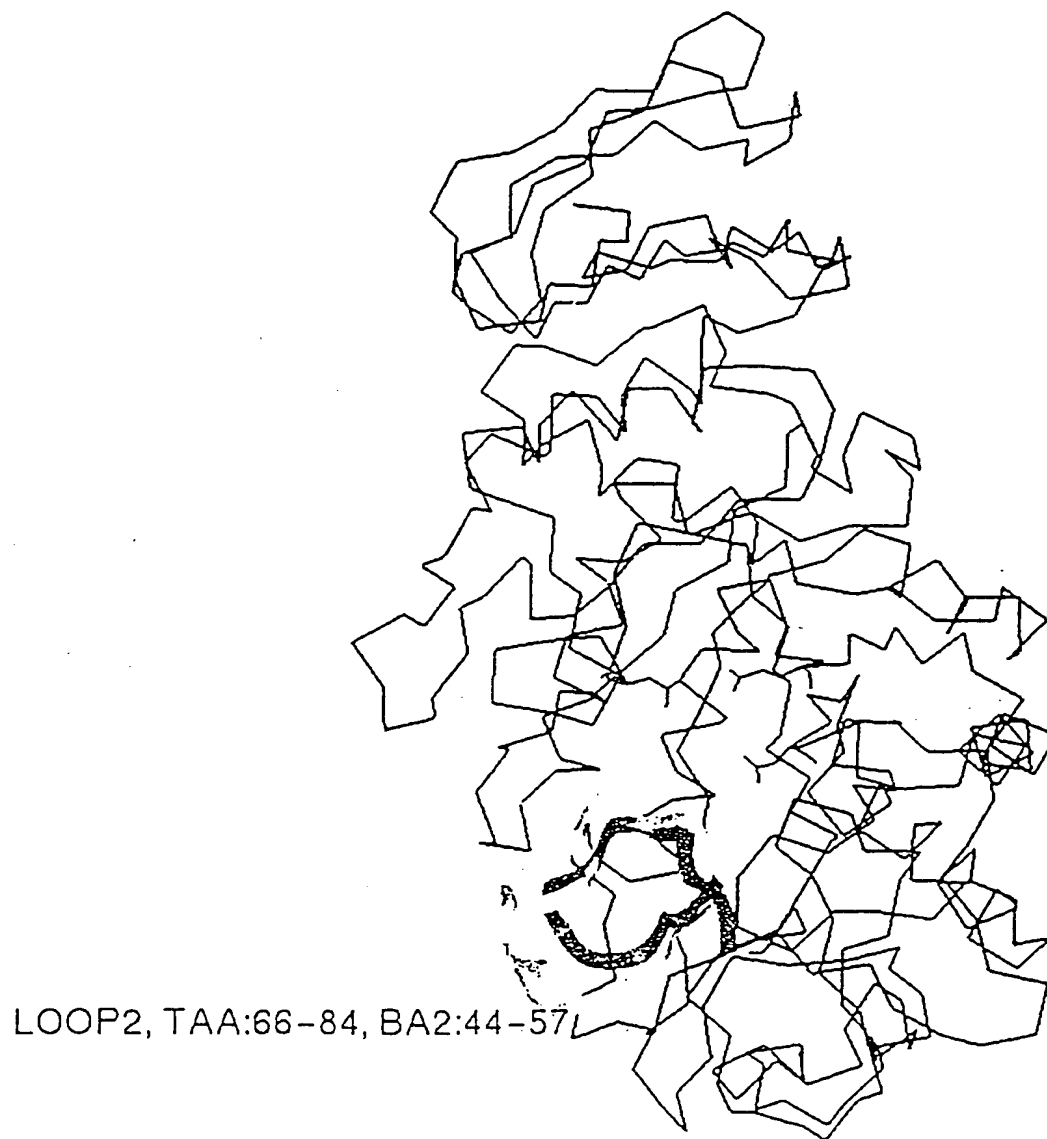


Fig. 1

2/11

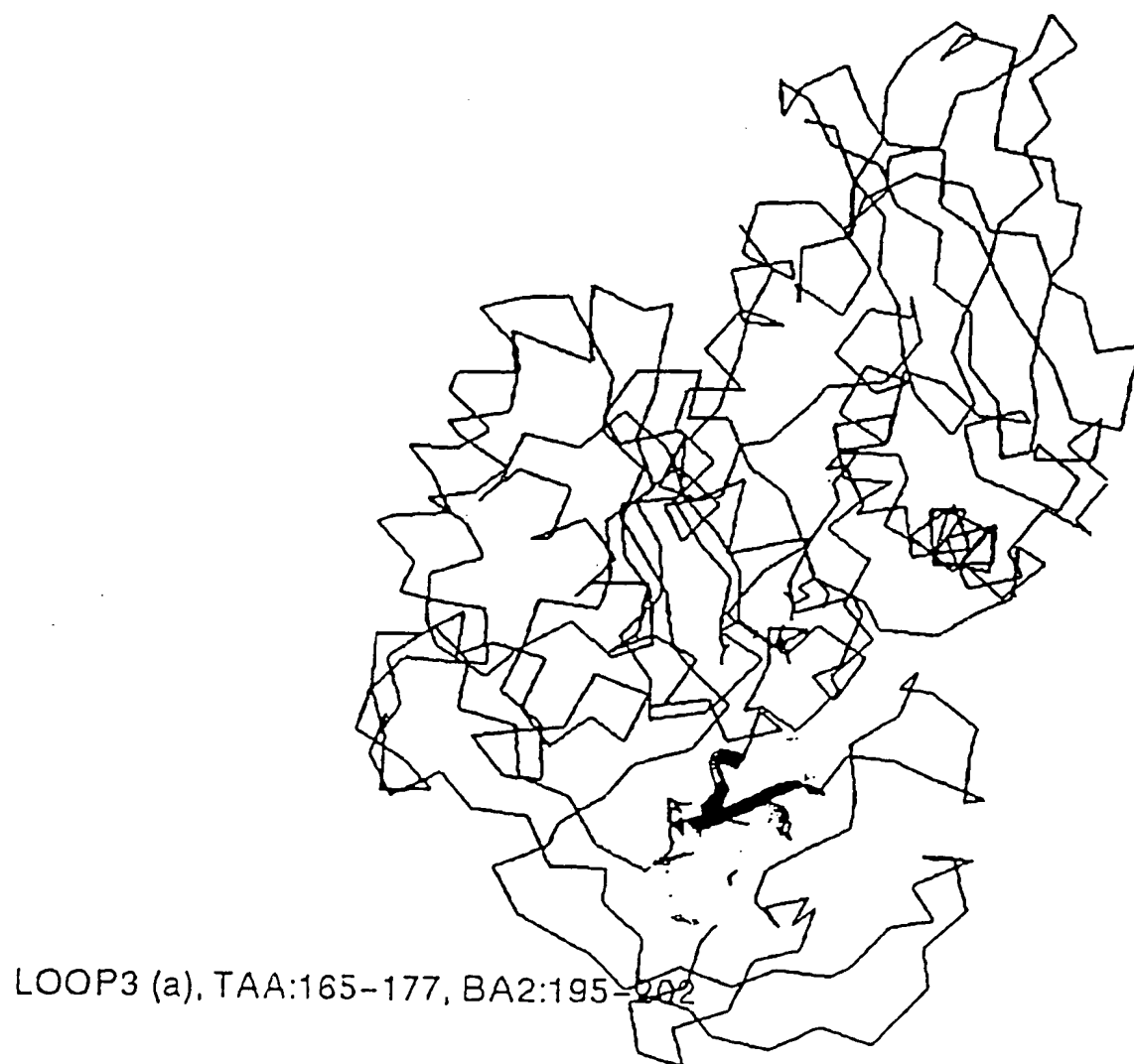


Fig. 2

3/11

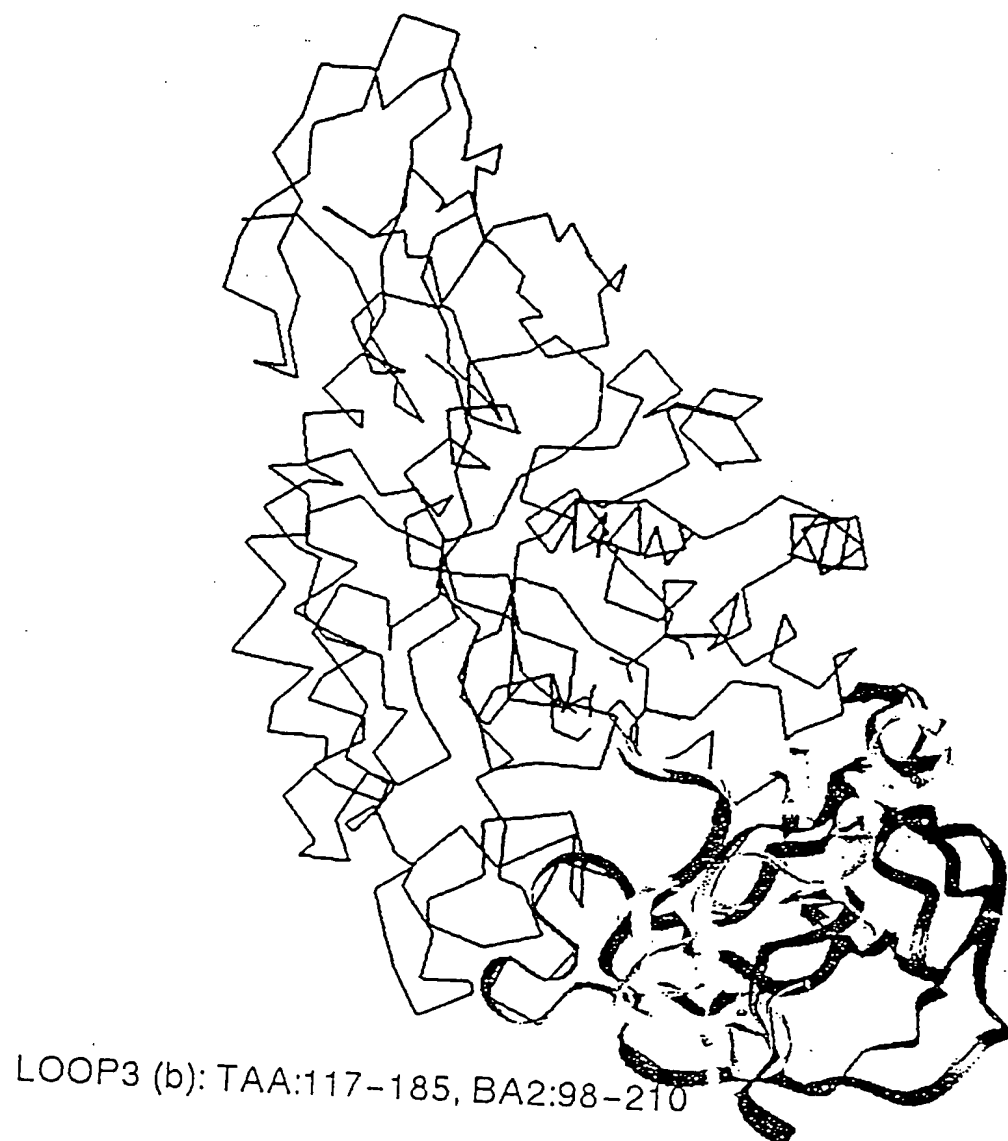


Fig. 3

4/11

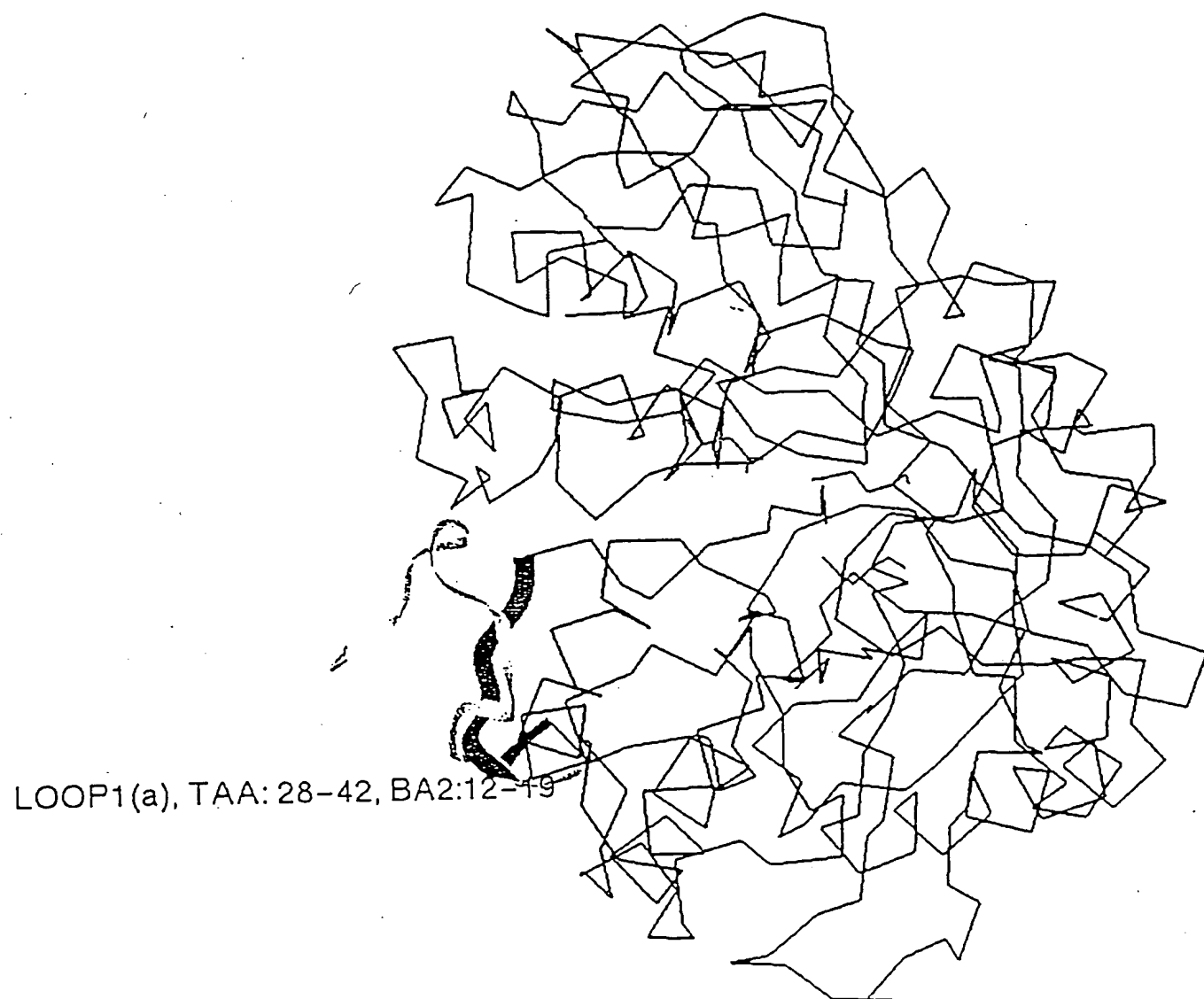


Fig. 4

5/11

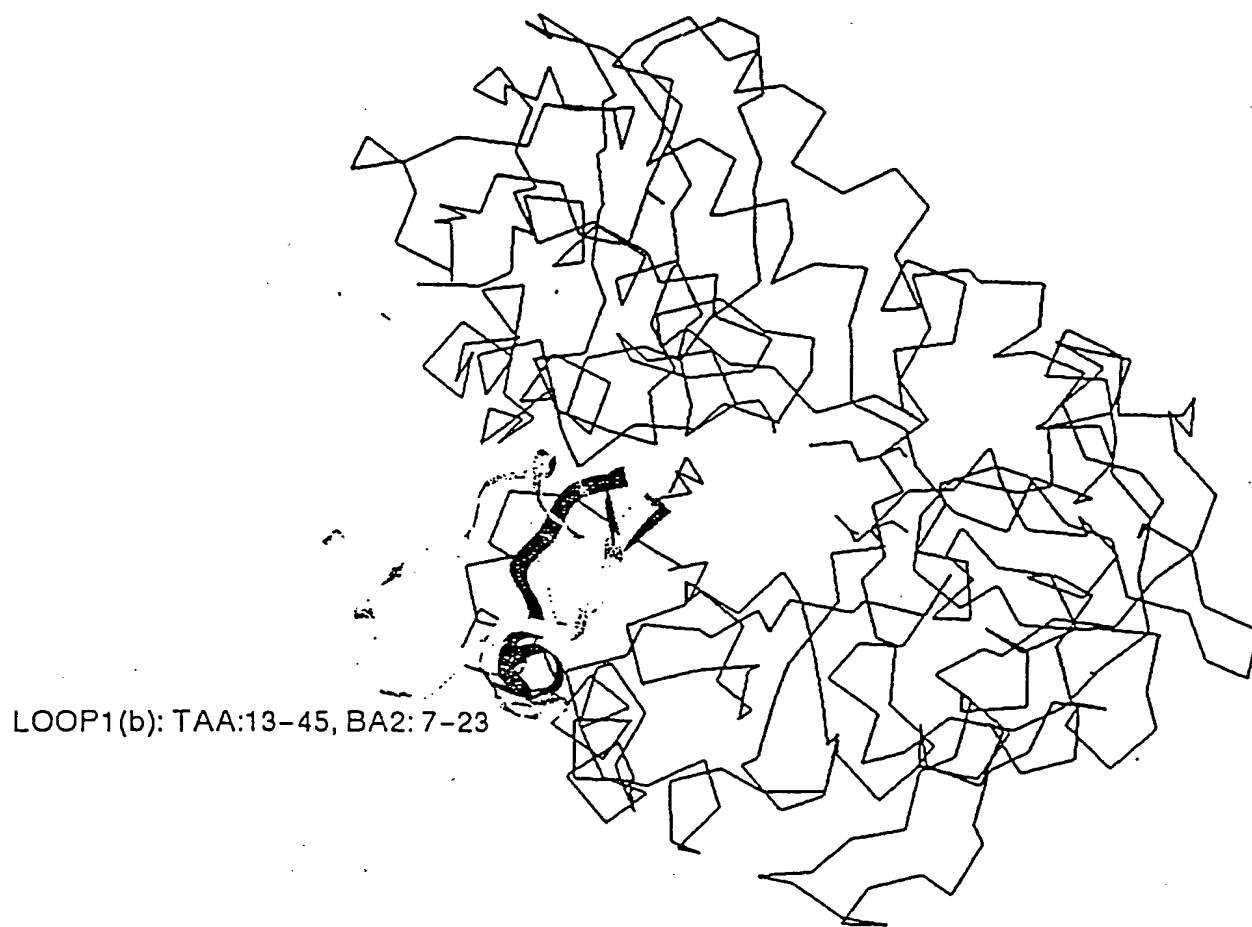


Fig. 5

6/11

LOOP8:TAA:291-313, BA2: 322-346

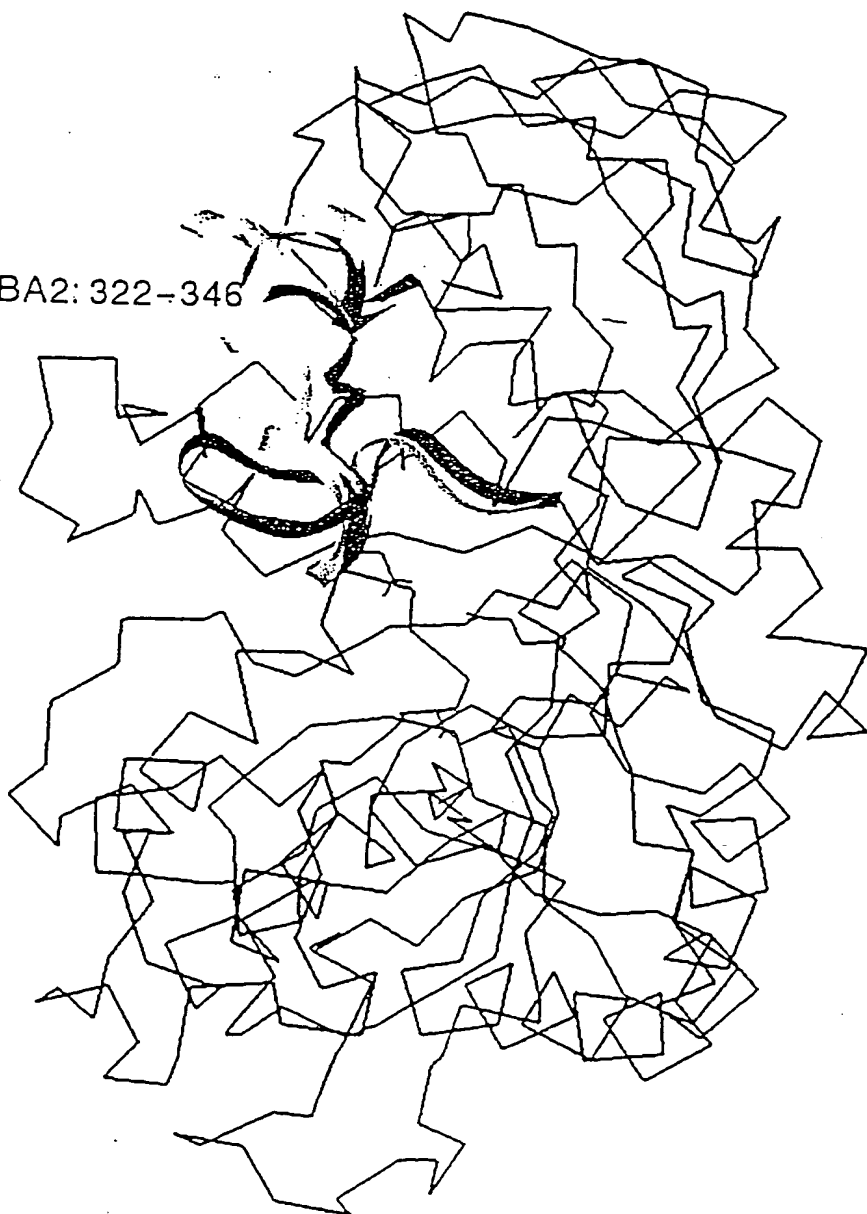


Fig. 6

7/11

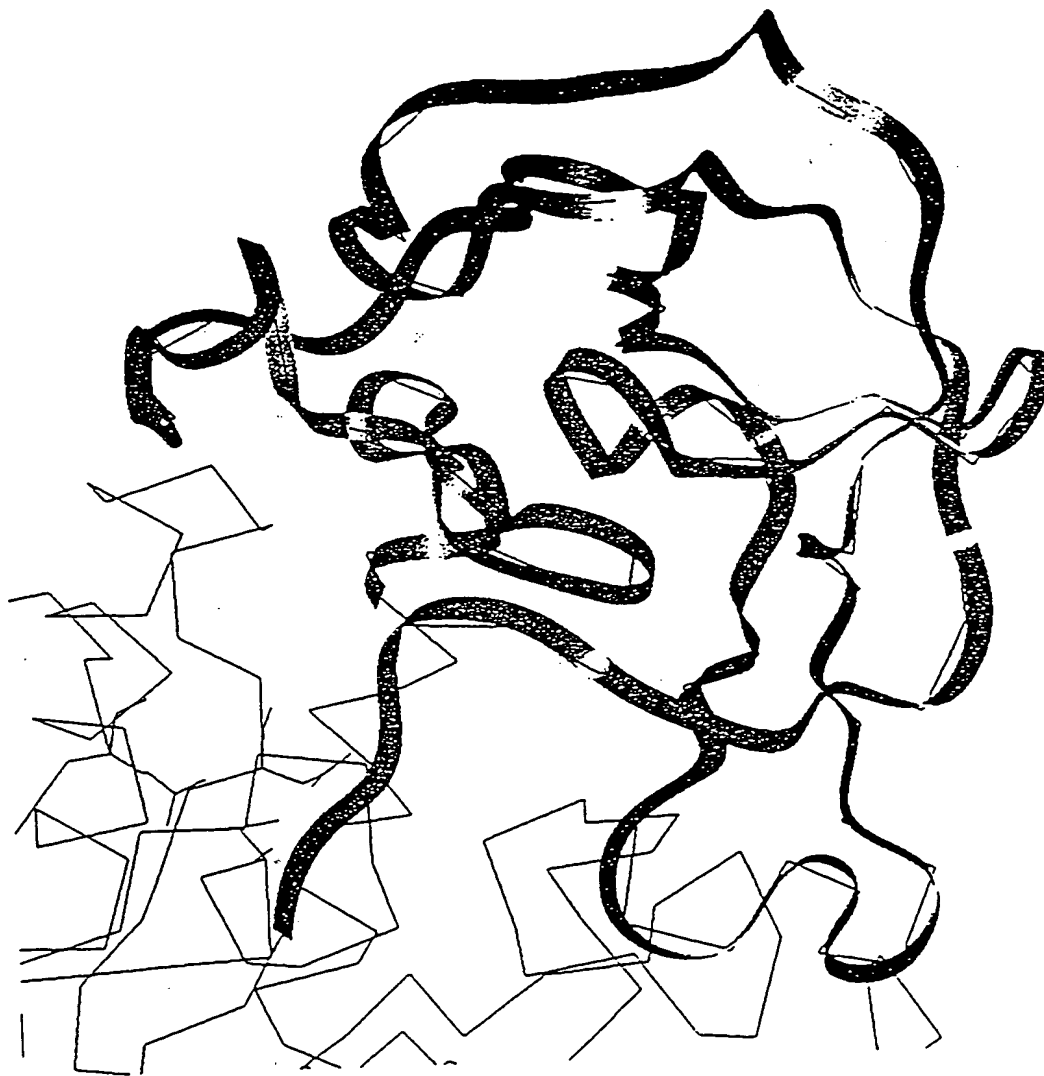


Fig. 7

8/11

1
CAT CAT AAT GGA ACA AAT GGT ACT ATG ATG CAA TAT TTC GAA TGG TAT TTG CCA AAT GAC
H H N G T N G T M M Q Y F E W Y L P N D

21
GGG AAT CAT TGG AAC AGG TTG AGG GAT GAC GCA GCT AAC TTA AAG AGT AAA GGG ATA ACA
G N H W N R L R D D A A N L K S K G I T

41
GCT GTA TGG ATC CCA CCT GCA TGG AAG GGG ACT TCC CAG AAT GAT GTA GGT TAT GGA GCC
A V W I P P A W K G T S Q N D V G Y G A

61
TAT GAT TTA TAT GAT CTT GGA GAG TTT AAC CAG AAG GGG ACG GTT CGT ACA AAA TAT GGA
Y D L Y D L G E F N Q K G T V R T K Y G

81
ACA CGC AAC CAG CTA CAG GCT GCG GTG ACC TCT TTA AAA AAT AAC GGC ATT CAG GTA TAT
T R N Q L Q A A V T S L K N N G I Q V Y

101
GGT GAT GTC GTC ATG AAT CAT AAA GGT GGA GCA GAT GGT ACG GAA ATT GTA AAT GCG GTA
G D V V M N H K G G A D G T E I V N A V

121
GAA GTG AAT CGG AGC AAC CGA AAC CAG GAA ACC TCA GGA GAG TAT GCA ATA GAA GCG TGG
E V N R S N R N Q E T S G E Y A I E A W

141
ACA AAG TTT GAT TTT CCT GGA AGA GGA AAT AAC CAT TCC AGC TTT AAG TGG CGC TGG TAT
T K F D F P G R G N N H S S F K W R W Y

161
CAT TTT GAT GGG ACA GAT TGG GAT CAG TCA CGC CAG CTT CAA AAC AAA ATA TAT AAA TTC
H F D G T D W D Q S R Q L Q N K I Y K F

181
AGG GGA ACA GGC AAG GCC TGG GAC TGG GAA GTC GAT ACA GAG AAT GGC AAC TAT GAC TAT
R G T G K A W D W E V D T E N G N Y D Y

201
CTT ATG TAT GCA GAC GTG GAT ATG GAT CAC CCA GAA GTA ATA CAT GAA CTT AGA AAC TGG
L M Y A D V D M D H P E V I H E L R N W

221
GGA GTG TGG TAT ACG AAT ACA CTG AAC CTT GAT GGA TTT ACA ATA GAT GCA GTG AAA CAT
G V W Y T N T L N L D G F R I D A V K H

241
ATA AAA TAT AGC TTT ACG AGA GAT TGG CTT ACA CAT GTG CGT AAC ACC ACA GGT AAA CCA
I K Y S F T R D W L T H V R N T T G K P

261
ATG TTT GCA GTG GCT GAG TTT TGG AAA AAT GAC CTT GGT GCA ATT GAA AAC TAT TTG AAT
M F A V A E F W K N D L G A I E N Y L N

281
AAA ACA AGT TGG AAT CAC TCG GTG TTT GAT GTT CCT CTC CAC TAT AAT TTG TAC AAT GCA
K T S W N H S V F D V P L H Y N L Y N A

Fig. 8

9/11

301

TCT AAT AGC GGT GGT TAT TAT GAT ATG AGA AAT ATT TTA AAT GGT TCT GTG GTG CAA AAA
S N S G G Y Y D M R N I L N G S V V Q K

321

CAT CCA ACA CAT GCC GTT ACT TTT GTT GAT AAC CAT GAT TCT CAG CCC GGG GAA GCA TTG
H P T H A V T F V D N H D S Q P G E A L

341

GAA TCC TTT GTT CAA CAA TGG TTT AAA CCA CTT GCA TAT GCA TTG GTT CTG ACA AGG GAA
E S F V Q Q W F K P L A Y A L V L T R E

361

CAA GGT TAT CCT TCC GTA TTT TAT GGG GAT TAC TAC GGT ATC CCA ACC CAT GGT GTT CCG
Q G Y P S V F Y G D Y Y G I P T H G V P

381

GCT ATG AAA TCT AAA ATA GAC CCT CTT CTG CAG GCA CGT CAA ACT TTT GCC TAT GGT ACG
A M K S K I D P L L Q A R Q T F A Y G T

401

CAG CAT GAT TAC TTT GAT CAT CAT GAT ATT ATC GGT TGG ACA AGA GAG GGA AAT AGC TCC
Q H D Y F D H H D I I G W T R E G N S S

421

CAT CCA AAT TCA GGC CTT GCC ACC ATT ATG TCA GAT GGT CCA GGT GGT AAC AAA TGG ATG
H P N S G L A T I M S D G P G G N K W M

441

TAT GTG GGG AAA AAT AAA GCG GGA CAA GTT TGG AGA GAT ATT ACC GGA AAT AGG ACA GGC
Y V G K N K A G Q V W R D I T G N R T G

261

ACC GTC ACA ATT AAT GCA GAC GGA TGG GGT AAT TTC TCT GTT AAT GGA GGG TCC GTT TCG
T V T I N A D G W G N F S V N G G S V S

481

GTT TGG GTG AAG CAA TAA
V W V K Q

Fig. 8 (cont.)

10/11

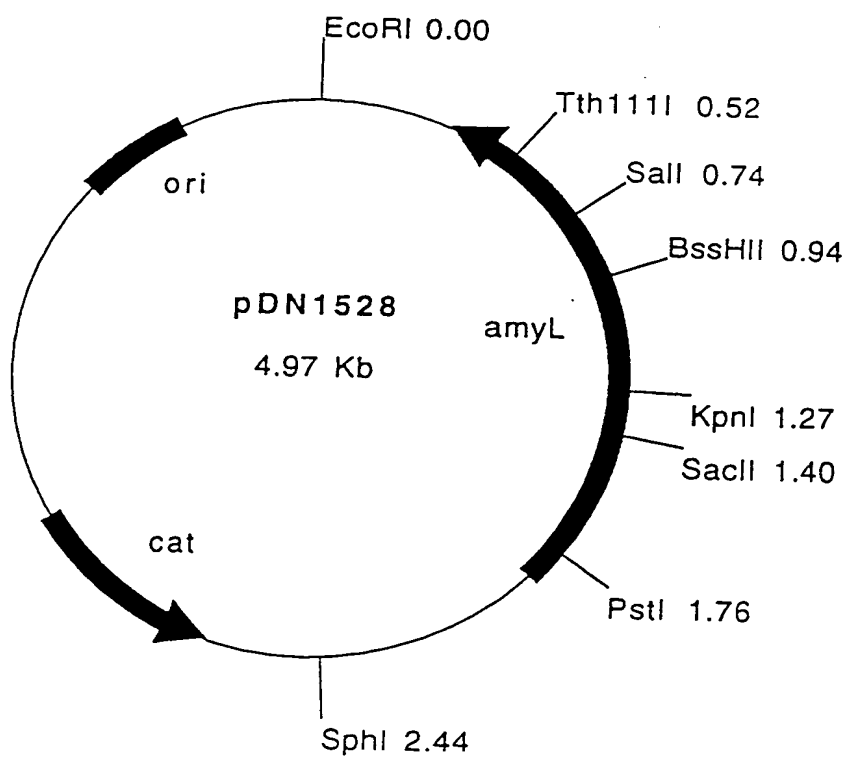


Fig. 9

11/11

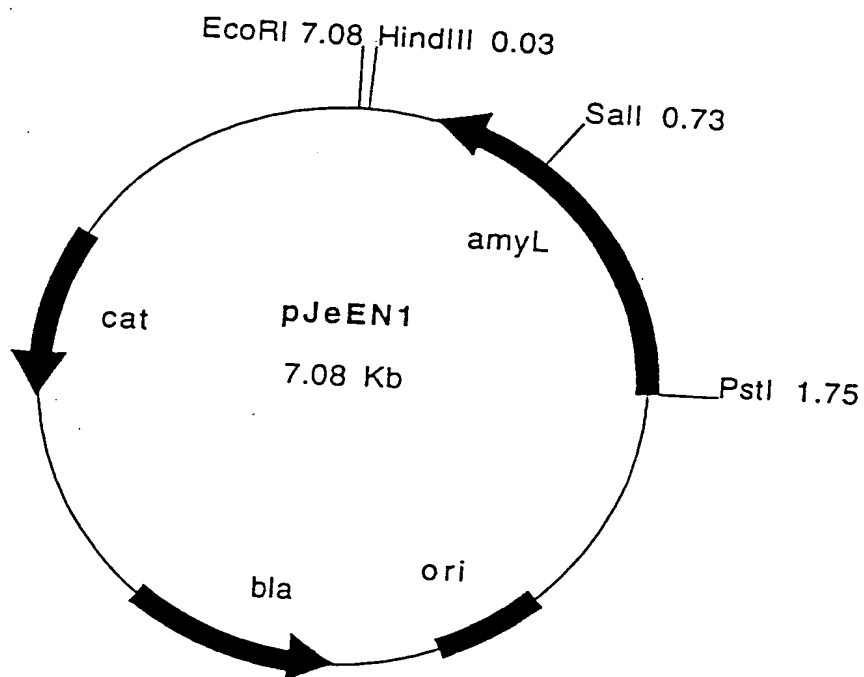


Fig. 10

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

A. CLASSIFICATION OF SUBJECT MATTER

IPC6: C12N 9/28, C12N 15/56

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC6: C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPI, CA, MEDLINE, BIOSIS

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	Dialog Information Services, File 5, BIOSIS PREVIEWS, Dialog accession no. 11619266, BIOSIS no. 98219266, Machius M et al: "Crystal structure of calcium-depleted Bacillus licheni- formis alpha-amylase at 2.2 A resolution", & Journal of Molecular Biology 246 (4). 1995. 545-559 --	1-17
X	Dialog Information Services, file 155, MEDLINE, Dialog accession no. 08974640, MEDLINE accession no. 94289640, Svensson B: "Protein engineering in the alpha-amylase family: catalytic mechanism, substrate specificity, and stability", & Plant Mol Biol (NETHERLANDS) May 1994, 25 (2) p141-57 --	1-17

☒ Further documents are listed in the continuation of Box C.☒ See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search

5 July 1996

Date of mailing of the international search report

05 -07- 1996

Name and mailing address of the ISA

Swedish Patent Office

Box 5055, S-102 42 STOCKHOLM

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Authorized officer

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The invention claimed relates to a method of constructing alpha-amylase variants with predetermined properties by comparing the three-dimensional structures of enzymes. The claims also include many alpha-amylase variants.

"A search for a special technical feature" as mentioned in PCT Rule 13.2 among the independent claims did not reveal a unifying, novel technical feature.

Accordingly, the following inventions were found:

- I Claims 1-17 focus on a method of constructing alpha-amylase variants by comparing the three-dimensional structure of a parent enzyme (Ternary-like alpha-amylase) with another enzyme e.g. mammalian or fungal alpha-amylases. The differences in structure are compared with the differences in function, whereafter new variants with new predictable characteristics are produced.
- II Claims 45-46 directed to a alpha-amylase variant that has decreased Ca^{2+} dependency,
- III Claim 47 directed to a alpha-amylase variant that exhibits higher activity below the pH-optimum than the parent enzyme.
- IV Claim 48 directed to a alpha-amylase variant having an increased thermostability and/or altered temperature optimum.
- V Claim 50 directed to a variant having reduced capability of cleaving an oligo-saccharide substrate close to its branching point.

Due to the complex construction of the claims and the fact that the search so far has not covered all aspects of the invention, it may be that further non-unity remarks can appear. If further searches are done, references might appear which will give further a posteriori non-unity remarks.

Therefore, the search has been restricted to the first invention.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	Dialog Information Services, file 155, MEDLINE. Dialog accession no. 08958150, MEDLINE accession no. 94273150, Nakatani H et al: "Effect of modifying histidine residues on the action of Bacillus amylo-liquefaciens and barley-malt alpha-amylases", & Carbohydr Res (NETHERLANDS) Apr 16 1994, 257 (1) p 155-61	1-17
Y	--	45-46
X	J. MED. BIOL., Volume 229, 1993, C. Chang et al, "Crystallization and Preliminary X-ray Crystallographic Analysis of alpha-Amylase from Bacillus subtilis" page 235 - page 238	1-17
A	WO 9100343 A2 (GIST-BROCADES N.V.), 10 January 1991 (10.01.91)	1-17
A	EP 0410498 A2 (GIST-BROCADES N.V.), 30 January 1991 (30.01.91)	1-17
A	JOURNAL OF BACTERIOLOGY, Volume 166, No 2, May 1986, G. L. Gray et al, "Structural Genes Encoding the Thermophilic alpha-Amylases of Bacillus stearothermophilus and Bacillus licheniformis" page 635 - page 643	1-17
P,X	WO 9535382 A2 (GISTBROCADES B.V.), 28 December 1995 (28.12.95), claims 1-2, abstract	45-46
Y	WO 9418314 A1 (GENENCOR INTERNATIONAL), 18 August 1994 (18.08.94)	45-46

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

Claims 18-43 are directed to a number of different variants that are composed of several inventions. They are, however, so complex and broad that no meaningful search can be done, especially as no special characteristic is linked to the groups of variants. It is for example unlikely that claim 18 concerns one invention. It is not believable that a change in any amino acid in one fragment for one/or none of the amino acids in a fragment of another enzyme gives an enzyme with the same new and valuable characteristic. The formulation of claims 18-43 is so complicated because of all the different combinations of amino acid substitutions.

Thus they do not comply with Art. 6. PCT prescribing that claims shall be clear and concise.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	Chemical Abstracts, Volume 108, No 11, 14 March 1988 (14.03.88), (Columbus, Ohio, USA), Buisson, G. et al, "Three dimensional structure of porcine pancreatic alpha-amylase at 2.9 Å resolution. Role of calcium in structure and activity", page 325, THE ABSTRACT No 90927h, EMBO J. 1987, 6 (13), 3909-3916 --	45-46
Y	Chemical Abstracts, Volume 112, No 15, 9 April 1990 (09.04.90), (Columbus, Ohio, USA), Vihinen, Mauno et al, "Site-directed mutagenesis of a thermostable alpha-amylase from Bacillus stearothermophilus: putative role of three conserved residues", page 347, THE ABSTRACT No 135178r, J. Biochem 1990, 107 (2), 267-272 --	45-46
A	US 4600693 A (KAREN L. KINDLE ET AL), 15 July 1986 (15.07.86) --	45-46
A	Chemical Abstracts, Volume 112, No 19, 7 May 1990 (07.05.90), (Columbus, Ohio, USA), Holm, Liisa et al, "Random mutagenesis used to probe the structure and function of Bacillus stearothermophilus alpha-amylase", page 351, THE ABSTRACT No 174785f, Protein Eng. 1990, 3 (3), 181-191 -- -----	45-46

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK96/00057

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

see next sheet

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see next sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☒ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
Claims 1-17 directed to a method of constructing alpha-amylase variants
and claims 45-46 directed to an alpha-amylase.
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐

The additional search fees were accompanied by the applicant's protest.

☒

No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

Information on patent family members

01/04/96

International application No.

PCT/DK 96/00057

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
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